Atlμs User's Guide

Version 7.3

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Introduction

This manual explains how to use Thermo Electron's OMNIC™ Atlμs™ software to perform automated data collection and spectral mapping experiments as well as image analysis with your microspectrometer system. You can automatically collect different types of compositional maps and display the collected data in a variety of formats. You can also create reports containing map data and print contour maps, 3-D displays, and comprehensive video images of the sample.

Before you begin working with the software, read the overview of automated data collection in the "Overview" chapter, which describes the main steps of performing an experiment. Then refer to the remaining chapters as you use the software. They describe in detail how to use the special windows and menu commands to collect and manipulate mapping data.

This manual covers only those features that are of special importance to OMNIC Atlμs. For information about standard OMNIC or OMNIC For Nicolet™ Almega™ features, choose OMNIC Help Topics from the Help menu. For information about optional OMNIC For Raman features, choose Raman Help Topics from the Raman menu (if present). For detailed information about using your microscope, motorized stage and video equipment, see the manuals or on-line documentation that came with each product.

For information about system requirements, see the document titled *Computer Requirements for Instruments Controlled by OMNIC Software* that came with your software.

Manual conventions

The following conventions are used in this manual to draw your attention to important information:

Note Notes contain helpful supplementary information. ▲

Important Follow instructions labeled "Important" to avoid damaging the system hardware or losing data. ▲

⚠ Caution Indicates a potentially hazardous situation which, if not avoided, may result in minor or moderate injury. It may also be used to alert against unsafe practices. ▲

⚠ Warning Indicates a potentially hazardous situation which, if not avoided, could result in death or serious injury. ▲

⚠ Danger Indicates an imminently hazardous situation which, if not avoided, will result in death or serious injury. ▲

Tips This symbol marks the start of a list of helpful tips for using the feature being discussed.

Starting OMNIC Atlμs

Follow these steps to start OMNIC Atlμs:

1. **Start Windows®.**

2. **Click the Start button on the Windows taskbar and then click All Programs (Programs in Windows 2000).**

3. **In the Thermo Nicolet folder, click the OMNIC program.**

   The OMNIC window appears with the Atlμs menu present in the menu bar. You can now define and collect a new map by using Show Atlμs Window in the Atlμs menu or open a stored map by using the Open in the File menu. See "The Atlμs window" in the "Preparing for Data Collection" chapter or "Opening a map or files from a split map" in the "Opening and Importing Map Data" chapter for details.

Note The first time you start OMNIC Atlμs, the Microscope Configuration dialog box appears allowing you to configure the microscope stage and other hardware. You will be able to change your settings later by using System Configuration in the Atlμs menu. See "Configuring the microscope" in the "Configuring the System" chapter for instructions for using this dialog box. ▲

About Z-axis initialization for Continuμm microscopes

If you have a Continuμm microscope with one of the optional automation packages, you can use OMNIC Atlμs to control stage movement along the Z-axis (up and down). Each time you turn on the Continuμm microscope power, the Z-axis position of the stage must be initialized before you can use OMNIC Atlμs to control movement of the stage in the Z dimension. Z-axis initialization is not completely automatic; you must take steps to protect the microscope hardware.

Follow these steps to initialize the Z-axis:

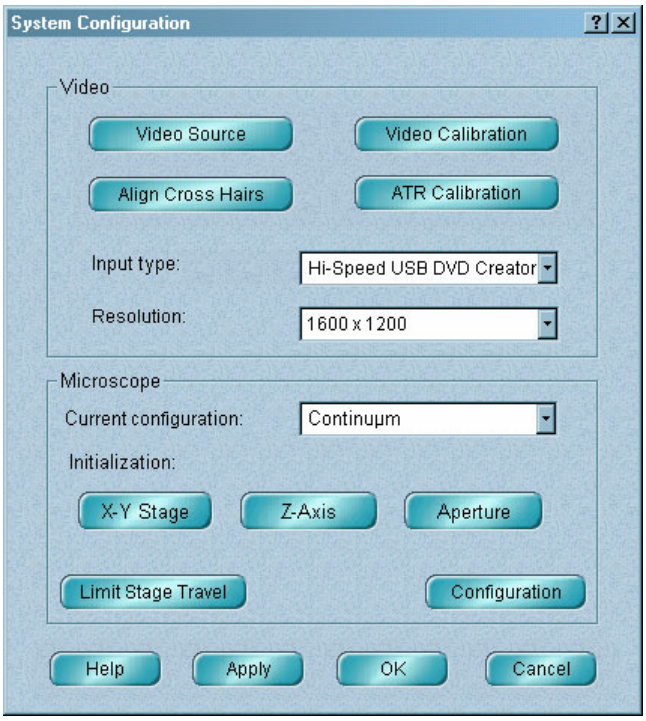
1. **Lower the condenser all the way and remove the nosepiece from the microscope.**

2. **Turn on the Continuμm microscope power.**

3. **Start OMNIC Atlμs.**

4. **Choose System Configuration from the Atlμs menu.**

   The System Configuration dialog box appears. Here is an example:



5. **Click the Z-Axis button and then follow the instructions that appear on the screen.**

Important To prevent damage to the microscope, make sure the condenser has been lowered all the way and the nosepiece has been removed from the microscope before initialization begins, as explained in the on-screen instructions. Do *not* choose OK (or Yes) before lowering the condenser and removing the nosepiece.
▲

- If you choose OK (or Yes) to initialize the Z-axis, the stage moves to its upper and lower limits and then back to the origin. The initialization takes a minute or two; a message is displayed until the process is complete. After initialization, the stage returns to its former position.

- If you cancel the initialization, a message informs you that all automation involving control of movement along the Z-axis has been disabled. This includes auto ATR contact, software control of Z-axis movement, and autofocus. Choose OK. If you want to use these features later, you must restart the microscope, start OMNIC Atlμs and then initialize the Z-axis.

6. **Reinstall the nosepiece.**

On-line Help

To see Help information about the unique OMNIC Atlμs features, choose Atlμs Help Topics from the Help menu. From the Help window that appears, you can display information about the feature of interest.

You can also use context-sensitive Help to display information:

- You can see information about many features in OMNIC Atlμs (such as a parameter in a dialog box) by clicking the feature using the *right* mouse button. (If the active dialog box or window includes a question mark button near the upper-right corner, you may need to first click that button and then click the feature of interest using the left mouse button.) A brief description of that feature appears along with a Discussion button or How To button, or both. (This type of Help may not appear for some features.) Click the Discussion button to see a more detailed discussion of the feature or dialog box. Click the How To button to see a step-by-step procedure for using the dialog box.

- To see information about a menu command, click the menu name to display the menu, use the down arrow key to highlight the name of the command, and then press the F1 function key. You can also press F1 when the dialog box or window for a command is displayed.

- If a dialog box or window contains a Help button, click it to see information about the features in the dialog box.

To see information about standard OMNIC features, choose OMNIC Help Topics from the Help menu. To see information about optional OMNIC For Raman features, choose Raman Help Topics from the Raman menu (if present). You can also use context-sensitive Help as explained above for both OMNIC and OMNIC For Raman features.

Exiting the software

Choose Exit from the File menu to exit OMNIC Atlμs.

Note You can also exit OMNIC Atlμs by clicking the OMNIC window's Close button (labeled "X") in the upper-right corner of the window. ▲

Questions or concerns

In case of emergency, follow the procedures established by your facility. If you have questions or concerns about safety or need assistance with operation, repairs or replacement parts, use the information below to contact Thermo Electron. Outside the U.S.A., contact the local Thermo Electron sales or service representative.

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Overview

This chapter provides an overview of collecting and working with microspectrometry data. It includes a summary of how to use OMNIC Atlμs to perform compositional mapping experiments, including automated point-of-interest analyses (at discrete sample points).

The software commands mentioned in this chapter are described in detail in later chapters.

Introduction to mapping

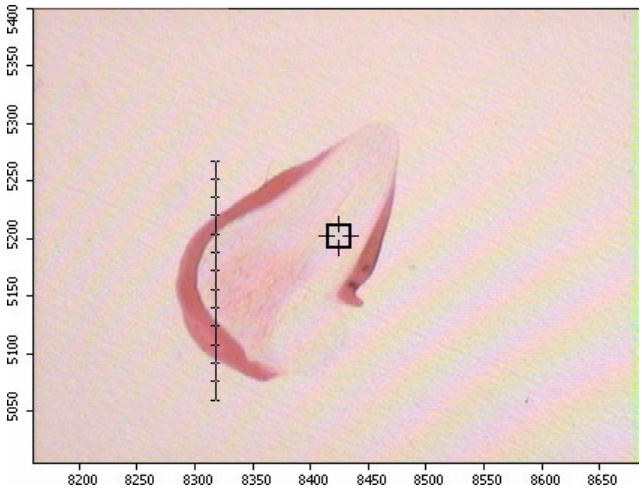
Compositional mapping in infrared, Raman and visible Raman microspectroscopy is a powerful analytical technique. By obtaining a series of spectra over a sample area, you can record the changes in the chemical composition of a sample and relate them to the visible image. Often, mapping is the only way that such detailed information can be obtained.

Mapping allows you to collect a large number of spectra quickly and automatically. By linking the parts of the mapping system—the microscope, motorized stage, video image and software—OMNIC Atlμs lets you efficiently analyze complex, microspectroscopic-size samples. Mapping performed using a Continuμm XL microscope with an array detector (also known as "imaging") lets you collect a map very quickly.

The three kinds of maps

You can use OMNIC Atlμs to collect three different types of maps: line maps (including line depth profiles), area maps (including area depth profiles), and maps consisting of data collected at discrete sample points (for example, discrete points in an ordered array). (Collecting a depth profile requires a visible Raman microscope.)

A *line map* consists of a series of spectra collected at sample points evenly spaced along a straight line on the sample. The following example shows the locations of the sample points for a line map.



The tick marks on the line indicate the locations of the sample points.

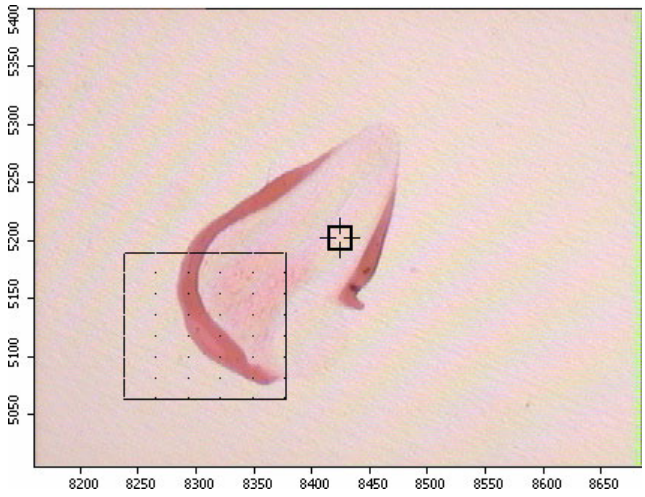
Line maps are useful for profiling across a boundary, such as a diffusion gradient of a solvent migrating across a polymer.

See “Setting up data collection” in the “Preparing for Data Collection” chapter or “Drawing a line map” in the “Preparing for Data Collection” chapter for complete information on specifying a line map.

Note Similar to a line map is a line depth profile, an evenly spaced series of spectra collected along a vertical axis within the sample using a visible Raman microscope. In this manual the term “map” includes depth profiles. See “Collecting a depth profile” in the “Collecting Data” chapter for more information. ▲

Note After data collection you can extract a line map from an area map, as explained in “Extracting a line map from an area map” in the “Processing and Analyzing Map Data” chapter. ▲

An *area map* is a series of spectra collected at sample points within a rectangular array. Here is an example showing the locations of the sample points for an area map.

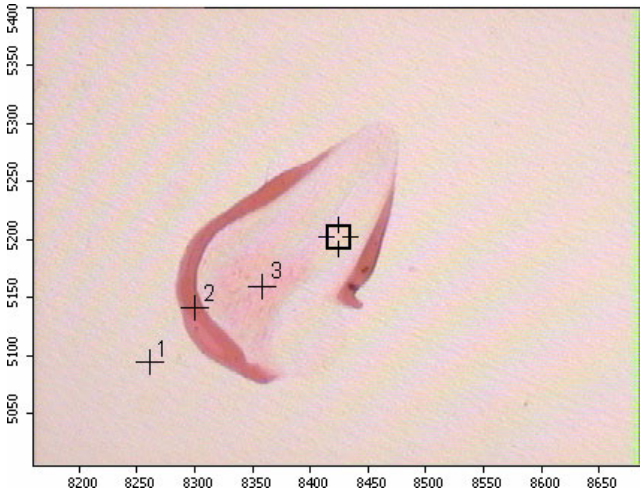


The dots indicate the locations of the sample points.

Area maps are most useful for compositional mapping of a discrete artifact within a sample, such as an inclusion in a film.

Note Similar to an area map is an area depth profile. This is created by collecting evenly spaced spectra along a series of evenly spaced vertical axes within the sample using a visible Raman microscope. See "Collecting a depth profile" in the "Collecting Data" chapter for more information. ▲

If a sample has one or several areas of interest, you can use OMNIC Atlμs to specify *discrete points* at which to collect spectra. Examples of this type of sample are scattered contaminants on a metal surface or a polymer film whose uniformity you want to measure. The following example shows some individually specified sample points. The points are labeled with consecutive numbers.



See “Specifying discrete points” in the “Preparing for Data Collection” chapter for complete information on specifying individual sample points.

You can also collect spectra of individual samples positioned in an ordered array, such as samples regularly spaced on a microscope slide. See “Specifying an ordered array” in the “Preparing for Data Collection” chapter for details.

Even the most routine FT-IR analysis of a single point of interest requires a sample point and a background point for a ratioed spectrum. (A background point is not needed for FT-Raman or visible Raman mapping experiments.) OMNIC Atlμs lets you easily specify these points by using the mouse or entering coordinates. The points you specify are labeled with consecutive numbers.

After you choose a map type, the next step in a mapping experiment is to define the area to be mapped (including the background location if needed) and set the data collection parameters. The map information is called a sequence and is part of the current experiment. You can save a sequence, and the rest of the experiment parameter settings, in an experiment file that can be opened later and used for other samples.

After the sequence is defined, you can collect the map. The software lets you display the collected data in several different ways, depending on what information about the sample is of interest. For example, you can display a contour map, with colors or lines representing different spectral intensities. You can also display individual spectra from a map.

See the "Preparing for Data Collection" chapter for complete information on specifying line maps, area maps, discrete sample points and depth profiles.

The importance of sample focus

One of the most important steps in any microspectroscopy experiment is properly presenting the sample to the microscope. For mapping experiments it is very important that the sample be level over the entire mapping region. If the sample is not level, the focus will change as the microscope stage moves different areas of the sample into the path of the beam. The spectra collected from areas that are not in focus could lead to baseline drifts, loss of spatial resolution and decreased signal-to-noise ratios.

Therefore, the first step in setting up a mapping experiment is to ensure that the sample is level on the microscope stage. If you cannot make the sample level over the entire mapping region, it will be necessary to refocus the stage before each spectrum is collected during the experiment. You can use Auto-Pause Before Each Spectrum (available through the Collect button on the Mapping tab of the Experiment Setup dialog box) to set the software to pause before collecting each spectrum so that you can adjust the focus. If you have the optional autofocus feature, you can use Autofocus At Each Map Point (All Map Types) (available through the Focus button on the Mapping tab of the Experiment Setup dialog box) to specify that the microscope be focused automatically before collecting each sample spectrum. See "Setting the focus parameters" in the "Preparing for Data Collection" chapter for details.

About autofocus

The optional autofocus feature lets you focus the microscope automatically using the focus buttons. When you initiate focusing with the buttons, the motorized autofocus equipment raises or lowers the stage (along the Z-axis) to bring the view of the sample surface into focus.

Note If you have the autofocus option, leave the Autogain switch (if present) on the video camera turned off unless you are performing a reflection experiment on a highly reflective substrate such as a gold mirror. ▲

On the Mapping tab of the Experiment Setup dialog box (available through Experiment Setup in the Collect menu), the Focus button lets you specify whether and how to focus the microscope automatically during data collection. See "Setting the focus parameters" in the "Preparing for Data Collection" chapter for details.

Note If you have a Centaurμs microscope with a motorized XL stage and the optional motorized Z-axis, you can use the Autofocus button in the Atlμs window. See "Using the focus buttons" in the "Preparing for Data Collection" chapter for more information. ▲

Tips for using autofocus

Autofocus operates by optimizing video image contrast as it moves the stage up and down. The maximum distance moved in either direction is 1.0 mm. If the system does not detect an optimum video image contrast, the software informs you that autofocus has failed. If you are performing a mapping experiment, the microscope continues to collect the map even if autofocus has failed.

Some low-contrast samples or samples with multiple focal planes (such as a sample in a diamond compression cell) can confuse the autofocus feature and cause a failure.

There are a number of things you can do to improve the system's autofocus performance and avoid failures:

- Bring the sample's vertical position to within 1.0 mm of correct focus. To do this, view the sample from the side (not through the eyepieces or on the video monitor) and raise or lower the stage to sharply focus the dot of white light hitting the sample surface.

- Adjust the illumination for optimum viewing. You should be able to see contrasting sample features. If the illumination is too high or too low, the autofocus feature will not be able to make use of contrast to optimize the focus.

- *If your microscope has field apertures, adjust them so that they are apparent in the field of view.* For difficult samples, first adjust the aperture so that its opening is completely within the field of view and then use autofocus. The edges of the aperture provide additional contrast that helps the system focus automatically.

Autofocus is generally successful when the above techniques are used. However, there are some notable samples that may still be difficult to focus:

- A sample with a perfectly smooth surface; for example, a new gold mirror. This sample is difficult because it has no sample features. A used gold mirror generally has a few imperfections that increase autofocus success.

- Highly diffuse samples. Samples that have multiple points of focus (paper, powder, etc.) generally cannot be focused automatically.

There is a way to overcome the limitations of autofocus for samples with poor contrast or with multiple points of focus: Use the Use Stored Focus Locations (Discrete Points Only) option to make use of stored focus positions. See "Focus parameters" in the "Preparing for Data Collection" chapter for details.

What is calibration?

When you use a video camera with a microscope, the magnification and field of view displayed on the video screen are different from what you see through the microscope eyepiece. When you change the microscope objective, the dimensions of the video system's field of view change. Because the video image is directly related to the stage position and magnification of the objective, there must be a way to tell the software the new size, in micrometers, of the video system's field of view so that the map can be defined correctly. This is known as calibrating the video image.

Your software provides a way to create and save calibrations for your different objectives. This lets you retrieve the appropriate video calibration when you change the objective, rather than having to recalibrate the video image.

The first time you use the software and microscope together, you are prompted to create a new calibration. (The prompt also appears when you choose Show Atlμs Window from the Atlμs menu if a calibration has not been performed.) Once a calibration has been created, the calibration used as the default when you start the software will be the last calibration selected the last time the software was run.

Note Whenever there is no current calibration for the video image, the stage will not function properly. Use the Video Calibration button in the System Configuration dialog box to calibrate the video image or to open a calibration. ▲

See "Calibrating the video image" in the "Configuring the System" chapter for complete information on creating and saving a calibration and opening a stored calibration.

Collecting backgrounds for FT-IR experiments

One or more background spectra are normally needed when you perform an infrared mapping experiment. It is very important that the background for a map be collected at the proper location. The background spectrum should not show any infrared absorptions but effectively compensate for any instrumental responses. A list of suggested background materials is provided in the section called "Collecting a background" in the "Collecting Data" chapter.

If your sample does not have an area suitable for collecting a background, you can collect one using a different material before setting up the sample for data collection. An example of this situation is a reflection-absorption experiment in which a background spectrum is collected using a separate mirror. The map will be ratioed against the last background you collected.

Important Background points remain defined in the map even after you have collected the background, so if the background point is on another sample, use Clear Map Sequence in the Edit menu before defining your new map. ▲

If your sample has a suitable background area, you can collect a background on the sample and use it to ratio the map sample spectra.

For information on specifying background points and collecting backgrounds, see "The tool palette" and "Background handling" in the "Preparing for Data Collection" chapter and "Collecting a background" in the "Collecting Data" chapter.

Using an aperture

You can use a rectangular aperture to define the sampling area for each point of a map (unless you are using a visible Raman microscope, or a Continuμm XL to perform an imaging experiment with the linear array). Rectangular apertures are variable; you can adjust the four sides to define the X and Y limits of any size area within the limits of the aperture (typically a range of 5 to 150 micrometers). You can also rotate the aperture to the desired angle up to 45 degrees in either direction. The same aperture size and orientation should be used for the background and the sample spectra in a map.

The aperture size should be large enough to provide enough signal through the microscope, but small enough to isolate the smallest area of interest in the mapping region. Sometimes a compromise between the two must be used.

Note If you have a Continuμm microscope with the automated Reflex™ aperture, you can use different aperture settings for the points in a discrete-point collection. The aperture is adjusted automatically at each point during the collection. See "Specifying discrete sample points" in the "Preparing for Data Collection" chapter for more information. ▲

Note A second, complementary way to define the smallest area of interest is by setting the step size (the distance between sample points). For example, you can distinguish changes in the mapped area to within 1 micrometer by using 1-micrometer steps, even though the aperture size may be 20 by 10 micrometers. ▲

See "Drawing an aperture," "Setting the automated Reflex aperture" and "Aperture parameters" in the "Preparing for Data Collection" chapter for more information on specifying apertures.

Note If you have a Continuµm XL microscope, use Scope Aperture on the Bench tab of the Experiment Setup dialog to specify aperturing. See "Setting the beam path for the Continuµm XL" in the "Preparing for Data Collection" chapter for details. You may wish to use a pre-aperture with this microscope; it works best for diffusely scattering samples. See your microscope documentation for more information. ▲

Performing an FT-IR or FT-Raman mapping experiment

An FT-IR or FT-Raman mapping experiment typically consists of some or all of the following main steps. See "Collecting ATR data with autofocus" in the "Collecting Data" chapter for procedures for collecting ATR data. See "Performing a visible Raman mapping experiment" if you have a Nicolet Almega system.

1. Position the sample on the stage and focus.
2. Specify the map sequence.
3. Set the data collection parameters.
4. Set the profile and display options. (This step is optional.)
5. Collect the map.

These steps are described later in this section. We refer you to the appropriate sections of this manual for complete information on using the needed software features.

Before you start

If you have not calibrated the video image for the microscope objective you will be using, calibrate it now. See "Calibrating the video image" in the "Configuring the System" chapter or "Selecting a calibration" in the "Preparing for Data Collection" chapter for more information.

If the Atlµs window is not displayed, choose Show Atlµs Window from the Atlµs menu before starting the following procedure.

In the general steps that follow we assume that a background can be collected using the sample. If this is not the case for your experiment, you can collect a background using an appropriate material before collecting the map. See "Using the tool palette" in the "Preparing for Data Collection" chapter for details on using the palette tools to specify a background point and "Collecting a map background" in the same chapter for information on collecting a background. *Use Clear Map Sequence in the Edit menu to clear the background point before specifying the map sequence.* Otherwise, a previously defined background point, if one exists, will be used.

Step 1: Position the sample on the stage and focus

Position the sample on the microscope stage so that it is perfectly level. If the sample cannot be made level over the entire mapping region, you will need to refocus the stage before each spectrum is collected during the experiment.

You can use Auto-Pause Before Each Spectrum (available through the Collect button on the Mapping tab of the Experiment Setup dialog box) to set the software to pause so that you can adjust the focus. See "Setting special mapping options" in the "Preparing for Data Collection" chapter for details.

If you have the optional autofocus feature, you can use Autofocus At Each Map Point (All Map Types) (available through the Focus button on the Mapping tab of the Experiment Setup dialog box) to specify that the microscope be focused automatically before collecting each sample spectrum. See "Setting the focus parameters" in the "Preparing for Data Collection" chapter for details.

Step 2: Specify the map sequence

Use the Atlμs window palette tools and the Mapping tab of the Experiment Setup dialog box to specify the map sequence. The map sequence defines the mapping region for the sample and includes information about the sample points, the background point, any aperture that is used and various option settings. See "Specifying a map sequence" and "Setting the data collection parameters for FT-IR and FT-Raman experiments" in the "Preparing for Data Collection" chapter for complete information.

You can also open a stored sequence if you previously created and saved one. To do this, open the experiment that contains the sequence by using the Experiment drop-down list box in the OMNIC window or the Open button in the Experiment Setup dialog box. (You can also open a sequence file using Open in the File menu.) If you open a sequence, skip to the next step unless you want to make changes to the sequence before collecting the map. See "Opening a map sequence" in the "Preparing for Data Collection" chapter for more information.

If you are performing an imaging experiment using the linear array detector of a Continuμm XL microscope, you can collect only an area map (not a line map or discrete point map) with the detector.

Step 3: Set the data collection parameters

Use Experiment Setup in the Collect menu to set the data collection parameters for data collection.

If you are using an infrared microscope, set Sample Compartment to Right μScope %T, Right μScope %R, Left μScope %T or Left μScope %R, depending on whether the microscope is installed to the left or right of the optical bench and whether you are performing a transmission or reflection experiment. Your setting positions the mirrors in the microscope and spectrometer for data collection.

If you are using an FT-Raman View Stage, the setting of Sample Compartment depends on the hardware you have. If you have the FT-Raman 960 spectrometer or the Magna-IR™ FT-Raman module, use the Main setting. If you have another model FT-Raman module, use the Raman setting.

Use the Collect tab in the Experiment Setup dialog box to set Final Format to the format that is appropriate for the kind of data you will be collecting. Set the other Collect parameters as appropriate for your experiment. See "Setting up data collection" in the "Preparing for Data Collection" chapter for details.

If you are performing an imaging experiment using the linear array detector of a Continuμm XL microscope, set Detector on the Bench tab to XL Array. This automatically sets Scope Aperture to Imaging.

Step 4: Set the profile and display options (optional)

If you are collecting a line map or area map, you can use the Mapping tab of the Experiment Setup dialog box to specify the type of profile to use for the map and the needed profile information. The default profile type setting is Chemigram™. See "Setting the profile parameters" in the "Preparing for Data Collection" chapter for more information.

You can specify how to display the collected line map or area map by using Options in the Edit menu. See "Setting the display options" in the "Preparing for Data Collection" chapter for more information.

Note This step is entirely optional. After you collect the map, you will be able to use Profile Setup in the Atlμs menu and Display Setup in the View menu to create profiles and change the display parameters. See "Creating a profile" in the "Processing and Analyzing Map Data" chapter and "Setting the display parameters" in the "Displaying Map Data" chapter for details. ▲

Step 5: Collect the map

To collect the map, choose Collect Map from the Collect menu and follow any instructions that appear on the screen. The collected map appears in a map window and you can begin working with it.

See "Collecting an FT-IR or FT-Raman map" in the "Collecting Data" chapter for more information on collecting a map. See the "Displaying Map Data" chapter for complete information on manipulating data within a map window. See the "Processing and Analyzing Map Data" for instructions for processing the data.

Performing a visible Raman mapping experiment

A visible Raman mapping experiment typically consists of some or all of the following main steps. See “Performing an FT-IR or FT-Raman mapping experiment” if you have an FT-IR or FT-Raman system.

1. Position the sample on the stage and focus.
2. Specify the map sequence.
3. Set the data collection parameters.
4. Set the profile and display options. (This step is optional.)
5. Collect the map.

These steps are described later in this section. We refer you to the appropriate sections of this manual for complete information on using the needed software features.

Before you start

If you have not calibrated the video image for the microscope objective you will be using, calibrate it now. See “Calibrating the video image” in the “Configuring the System” chapter or “Selecting a calibration” in the “Preparing for Data Collection” chapter for more information.

If the Atlμs window is not displayed, choose Show Atlμs Window from the Atlμs menu before starting the following procedure.

Step 1: Position the sample on the stage and focus

Position the sample on the microscope stage so that it is perfectly level. If the sample cannot be made level over the entire mapping region, you will need to refocus the stage before each spectrum is collected during the experiment.

You can use Auto-Pause Before Each Spectrum (available through the Collect button on the Mapping tab of the Experiment Setup dialog box) to set the software to pause so that you can adjust the focus. See “Setting special mapping options” in the “Preparing for Data Collection” chapter for details.

If you have the optional autofocus feature, you can use Autofocus At Each Map Point (All Map Types) (available through the Focus button on the Mapping tab of the Experiment Setup dialog box) to specify that the microscope be focused automatically before collecting each sample spectrum. See “Setting the focus parameters” in the “Preparing for Data Collection” chapter for details.

Step 2: Specify the map sequence

Use the Atlμs window palette tools and the Mapping tab of the Experiment Setup dialog box to specify the map sequence. The map sequence defines the mapping region for the sample and includes information about the sample points and various option settings. See “Specifying a map sequence” and “Setting the data collection parameters for visible Raman experiments” in the “Preparing for Data Collection” chapter for complete information.

You can also open a stored sequence if you previously created and saved one. To do this, open the experiment that contains the sequence by using the Experiment drop-down list box in the OMNIC window or the Open button in the Experiment Setup dialog box. (You can also open a sequence file using Open in the File menu.) If you open a sequence, skip to the next step unless you want to make changes to the sequence before collecting the map. See “Opening a map sequence” in the “Preparing for Data Collection” chapter for more information.

Step 3: Set the data collection parameters

Use Experiment Setup in the Collect menu to set the data collection parameters for data collection.

Use the Collect tab in the Experiment Setup dialog box to set Final Format to the format that is appropriate for the kind of data you will be collecting. Set the other Collect parameters as appropriate for your experiment. See “Setting up data collection” in the “Preparing for Data Collection” chapter for details.

Step 4: Set the profile and display options (optional)

If you are collecting an area map or area depth profile, you can use the Mapping tab of the Experiment Setup dialog box to specify the needed profile information. The default profile type setting is Chemigram™. See “Setting the profile parameters” in the “Preparing for Data Collection” chapter for more information.

You can specify how to display the collected line map, area map or depth

profile by using Options in the Edit menu. See “Setting the display options” in the “Preparing for Data Collection” chapter for more information.

Note This step is entirely optional. After you collect the map, you will be able to use Profile Setup in the Atlμs menu and Display Setup in the View menu to create profiles and change the display parameters. See “Creating a profile” in the “Processing and Analyzing Map Data” chapter and “Setting the display parameters” in the “Displaying Map Data” chapter for details. ▲

Step 5: Collect the map

To collect the map, choose Collect Map from the Collect menu and follow any instructions that appear on the screen. The collected map appears in a map window and you can begin working with it.

See “Collecting a visible Raman map” in the “Collecting Data” chapter for more information on collecting a map. See the “Displaying Map Data” chapter for complete information on manipulating data within a map window. See the “Processing and Analyzing Map Data” for instructions for processing the data.

Configuring the System

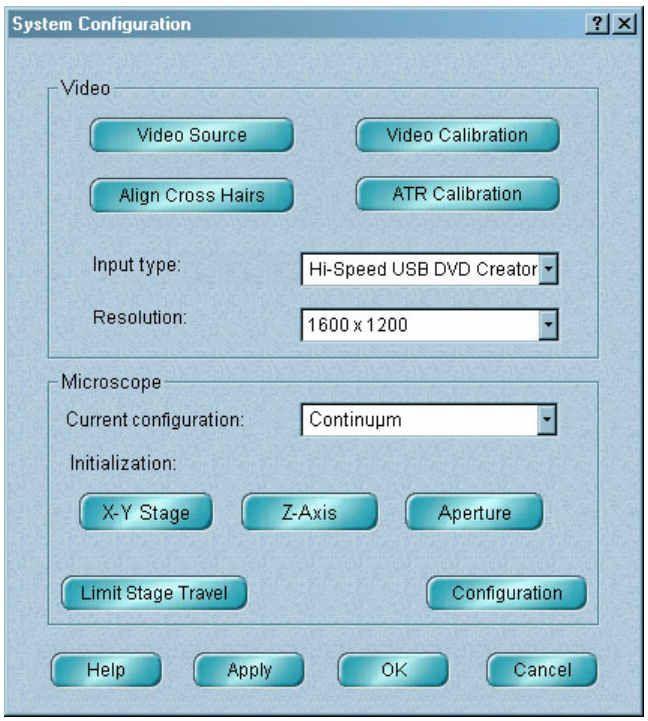
Before you collect map data for the first time, use System Configuration in the Atlμs menu to perform the following tasks:

- Specify how the video driver will display the video image.
- Calibrate the video image.
- Align the video cross hairs.
- Specify the type of camera hardware you are using.
- Specify the type of video input you are using.
- Specify your microscope configuration.
- Initialize the stage.
- Initialize the automated Reflex aperture, if present.
- Limit the stage travel.
- Configure the microscope.

Follow the general steps below to use the System Configuration command. The next sections provide detailed instructions for performing the operations listed above.

1. **Choose System Configuration from the Atlµs menu.**

   The System Configuration dialog box appears. Here is an example:



2. **Use the provided features as desired.**

   If you change any parameter settings in this dialog box, you can click the Apply button to see the effects of your changes without closing the dialog box.

   See the next sections for detailed instructions for using the provided features.

3. **Choose OK.**

Configuring the video

Use the features in the Video box in the System Configuration dialog box to do the following:

- Specify how the video driver will display the video image.
- Calibrate the video image.
- Align the video cross hairs.
- Specify the camera hardware you are using (except on Nicolet Almega systems).
- Specify the type of video input you are using.
- Specify the type of video connector you are using.

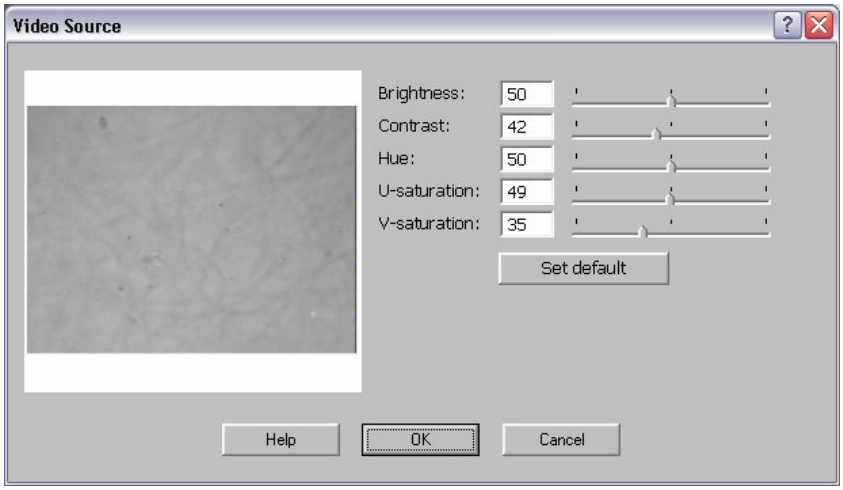
The next sections explain how to perform these tasks.

Setting the video source parameters

Use the Video Source button to specify how you want the video driver to display the video image. Follow these steps:

1. **Click the Video Source button in the System Configuration dialog box.**

   The Video Source dialog box appears. Here is an example:



   The features in this dialog box may vary depending on your frame grabber. See the documentation that came with the frame grabber for a description of the provided parameters.

Note You can also use many of the tools, such as the arrow tool, in the Atlμs window to display this dialog box. Simply click anywhere in the navigation pane or video pane, and then choose Video Source from the pop-up menu. ▲

2. **Set the parameters as desired.**

   To set a parameter, type a value in the text box or drag the indicator along the bar to the right of the text box. You can see the effects of your settings in the video image.

   To return all the parameters to their default settings, choose Set Default.

3. **Choose OK.**

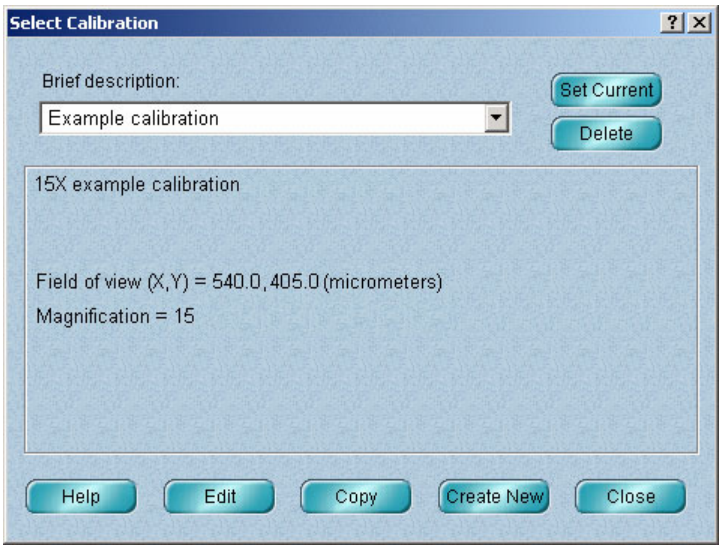
Video calibration

Use the Video Calibration button to select a saved calibration to use for the video pane or to create a new calibration. You can also delete a saved calibration.

Whenever the size of the video field of view changes (because you have changed the microscope objective), you need to select an appropriate calibration, or calibrate the video image, to coordinate what is displayed in the video pane with the actual field of view. That is, the number of micrometers displayed in the video pane must match the number of micrometers in the field of view. The calibration is very important. If the video image is not calibrated, any maps you define are invalid because the software is unable to map the correct region of interest.

See “What is calibration?” in the “Overview” chapter for more discussion of video image calibration.

When you choose Video Calibration, the Select Calibration dialog box appears showing the currently selected calibration and information about it:



The next sections explain how to create a new calibration and work with existing calibrations.

Note If you have a Nicolet Almega system, several default calibrations are provided and installed during calibration. You can delete those that do not apply to your system. See "Opening a saved calibration" for instructions for opening a calibration. See "Deleting a saved calibration" for instructions for deleting a calibration. ▲

Calibrating the video image

Follow these steps to calibrate the video image:

1. **Place a micrometer slide on the stage, and focus on the scale near the center of the slide.**

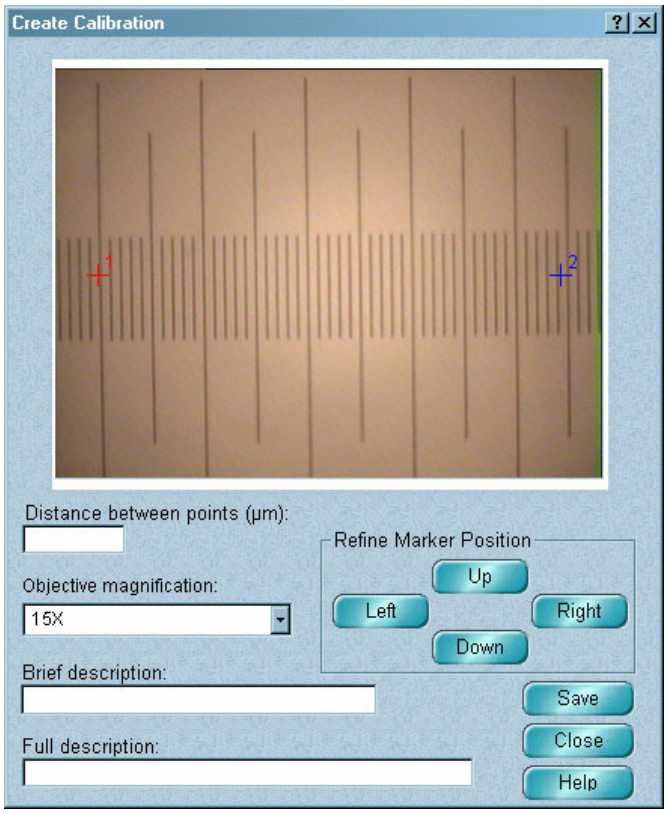
   You can use the provided pinhole if you don't have a micrometer slide. Focus on the edge of the pinhole.

   Use transmission illumination for this step.

   If you prefer, you can place the micrometer slide (or pinhole) on the stage and focus after step 2.

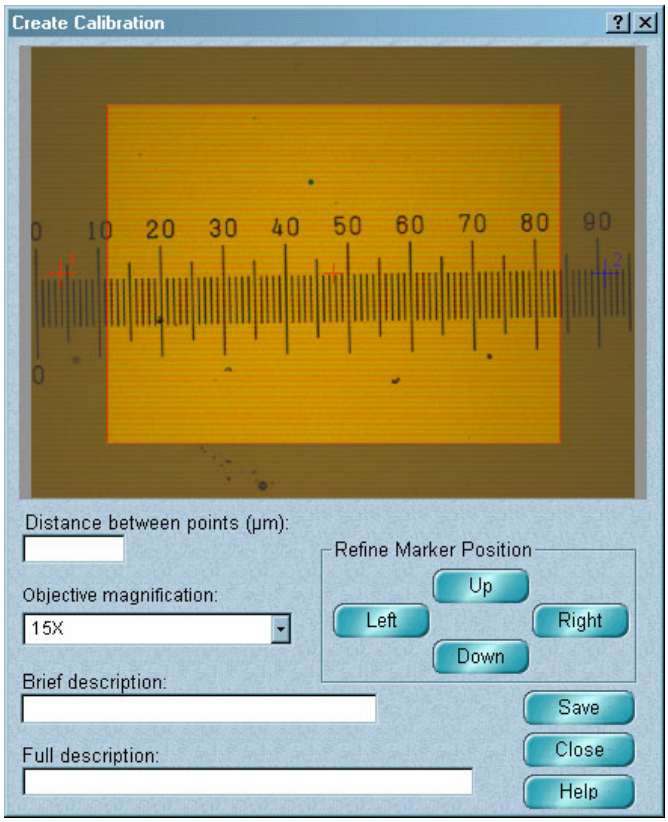
2. **Click the Create New button in the Select Calibration dialog box.**

   The Create Calibration window appears, displaying a video image and features for calibrating it. Here is an example showing the image from an analog camera:



Create Calibration window for analog camera

Here is an example showing the image from a digital camera:



Create Calibration window for digital camera

Notice that the digital camera image contains a lighter rectangular area in the center. Only this area will appear in the video pane of the Atlµs window and be used for capturing video images. By adjusting the size, shape and location of the area, you can eliminate distortions and uneven illumination that can occur around the perimeter of a video image. To adjust the size and shape of the area, drag its red border. To move the area, drag its center to the desired location.

To make it easier to see details in the analog or digital video image, you can enlarge the window by dragging its sides or corners.

3. **Drag the markers labeled "1" and "2" to division lines on the scale.**

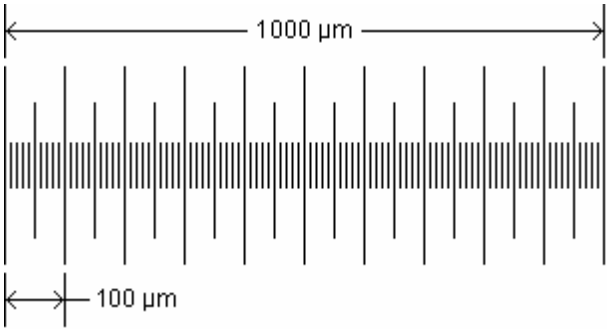
Important If you are using a digital camera, the markers must be within the lighter rectangular area. ▲

If you are using the pinhole, drag the markers to opposite sides of the hole so that the distance between them is the diameter of the hole.

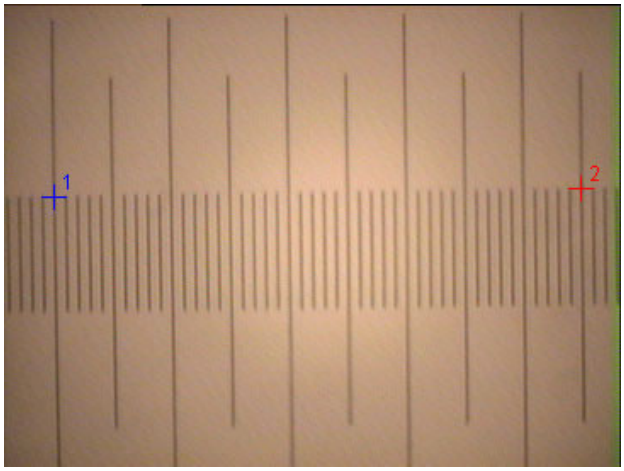
For best accuracy use division lines that are far apart.

You can use the buttons in the Refine Marker Position box to more finely adjust the position of the currently active (red) marker.

The illustration below shows the distances between major division lines. The distance between the minor division lines is 10 micrometers.



Here is an example showing the markers placed on major division lines that are 450 micrometers apart:



4. **Type the distance between the markers in micrometers in the Distance Between Points (µm) text box.**

5. **Select the magnification of the objective you are using from the Objective Magnification drop-down list box.**

   If you have an FT-Raman View Stage, select Fixed Objective.

6. **Type a brief description of the calibration in the Brief Description text box.**

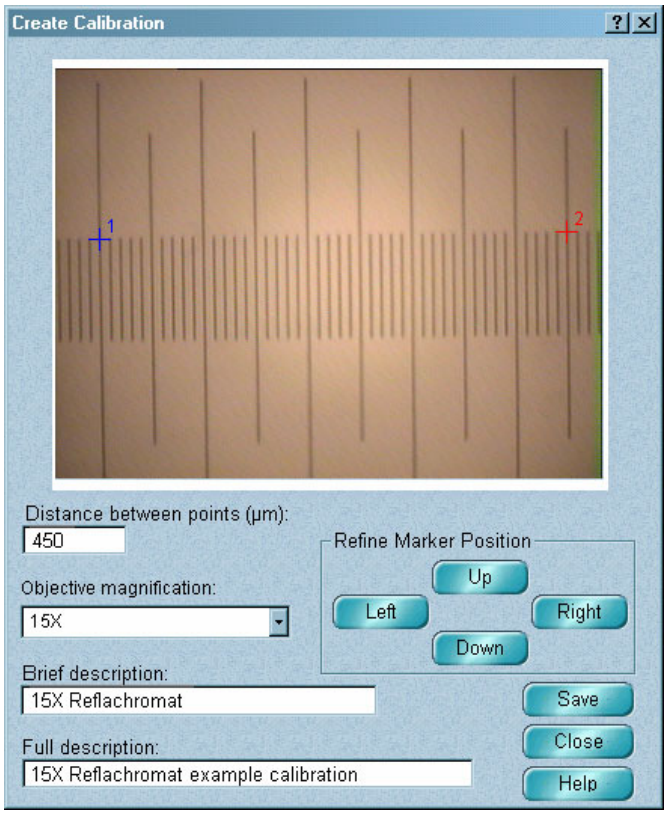
   This description will be listed in the Brief Description drop-down list box in the Select Calibration dialog box after you save the calibration.

7. **Type a more detailed description of the calibration in the Full Description text box.**

   The full description is a good way to record what the calibration was created for. It's helpful to include a description of the objective that was used for the calibration.

   After you save the calibration, the full description will appear in the Select Calibration dialog box when you select the calibration from the Brief Description drop-down list box.

Here is an example showing all of the information entered in the text boxes:



8. **Click the Save button.**

9. **Click the Close button.**

The saved calibration is now available for use. For more information see "Opening a saved calibration" in this chapter or "Selecting a calibration" in the "Preparing for Data Collection" chapter.

You can edit the saved calibration by using the Edit button in the Select Calibration dialog box. See "Editing a calibration" for details.

Tips Calibrating the video image

- To verify that the video image has been calibrated correctly, first select the calibration from the Brief Description drop-down list box in the Select Calibration dialog box, choose Set Current, choose Close to close the dialog box, and choose OK to close the System Configuration dialog box. Then use the stage movement tool to click a location in the video image in the Atlμs window. If that location moves to the center of the video pane, the video image has been calibrated correctly.

  You can also use the ruler tool and stage micrometer to verify the calibration: Use the ruler tool to measure the distance between two sample features. Position one of the features at the cross hairs and then use the stage micrometer to measure the distance traveled when you move the other feature to the cross hairs. The two measurements should be the same.

Opening a saved calibration

Follow these steps to open a saved calibration:

1. **Select the calibration to open from the Brief Description drop-down list box in the Select Calibration dialog box.**

   Information about the selected calibration appears below the drop-down list box. This information was entered when the calibration was created (see "Calibrating the video image").

2. **Click the Set Current button.**

   The calibration will be in effect when you next use the Atlμs window.

Note You can also use the Show Calibration Bar button in the Atlμs window to select a saved calibration. See "Selecting a calibration" in the "Preparing for Data Collection" chapter for details. ▲

Editing a saved calibration

Follow these steps to edit a saved calibration:

1. **Select the calibration to edit from the Brief Description drop-down list box in the Select Calibration dialog box.**

2. **Click the Edit button.**

   The Create Calibration window appears.

3. **Adjust the calibration as desired.**

   You can move the markers and change the information in the dialog box. If you are using a digital camera, you can adjust the size, shape and location of the lighter rectangular area. See "Calibrating the video image" for information about using the provided features.

4. **Click the Save button.**

5. **Click the Close button.**

Copying a saved calibration

If you want to create a calibration that is very similar to a saved calibration, you can copy the saved calibration and then make any needed changes. Follow these steps to copy a calibration:

1. **Select the calibration to copy from the Brief Description drop-down list box in the Select Calibration dialog box.**

2. **Click the Copy button.**

   A new calibration is added in the Brief Description drop-down list box, with the word "Copy" appended to the description.

Deleting a saved calibration

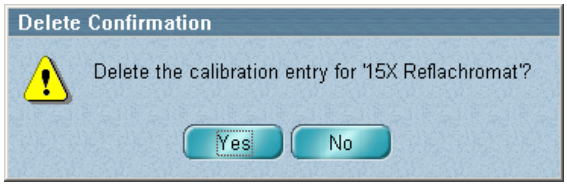
Follow these steps to delete a saved calibration:

1. **Select the calibration you want to delete from the Brief Description drop-down list box in the Select Calibration dialog box.**

   Information about the selected calibration appears below the drop-down list box. This information was entered when the calibration was created (see "Calibrating the video image").

2. **Click the Delete button.**

   A confirmation message appears. Here is an example:



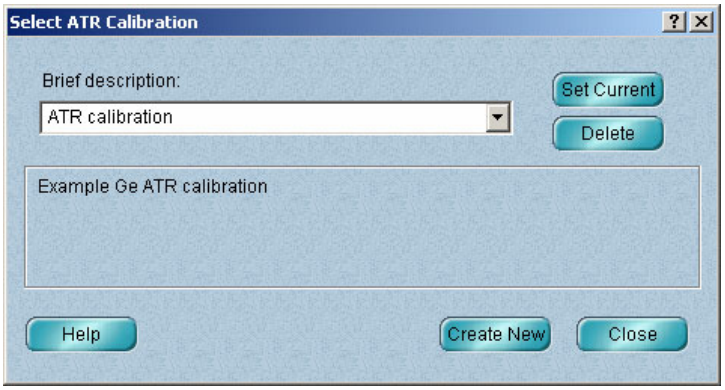
3. **Choose Yes.**

ATR calibration

Use the ATR Calibration button to select a saved calibration to use for ATR images or to create a new ATR calibration. You can also delete a saved ATR calibration.

An ATR calibration compensates for any difference between the apparent location of a point in an ATR image displayed in the video pane and the location of the point as seen through the microscope eyepieces.

When you choose ATR Calibration, the Select ATR Calibration dialog box appears showing the currently selected calibration and information about it:



The next sections explain how to create a new ATR calibration and work with existing ATR calibrations.

Performing an ATR calibration

Follow these steps to perform an ATR calibration:

1. **Prepare the system for ATR operation.**

   The required preparations may vary depending on your microscope model. An ATR objective should be installed, and the software should be set for ATR data collection. For example, select Auto ATR Contact in the Focus dialog box if it is available (see "Setting the focus parameters" in the "Preparing for Data Collection" chapter).

2. **Apply a thin coating of carbon soot to a glass slide.**

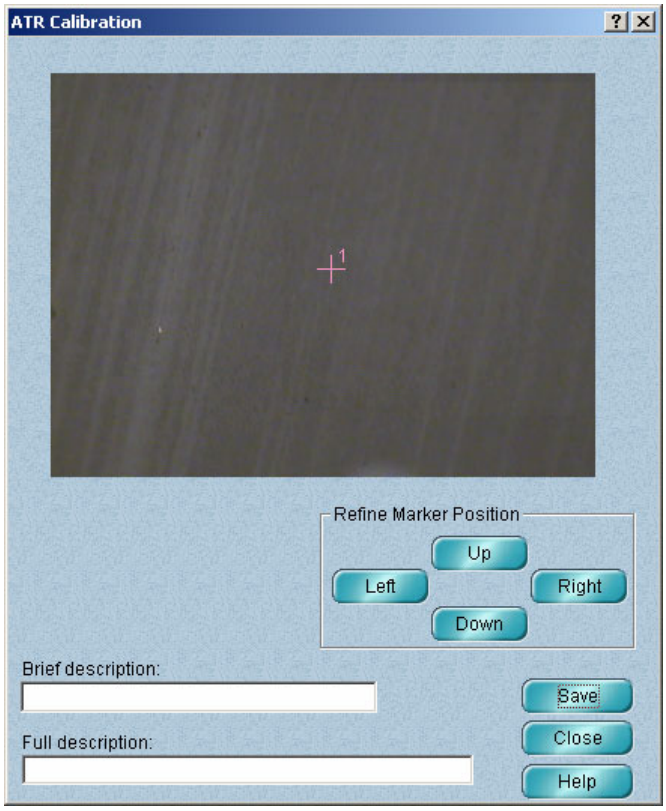
   An easy way to do this is to light a match or candle, hold the slide at one end, and briefly allow the flame to touch one side of the slide near the center.

3. **Place the slide on the stage with the soot-coated side facing up.**

4. **With the ATR crystal out of the beam path, focus on the soot.**

5. **Click the Create New button in the Select Calibration dialog box.**

   The ATR Calibration window appears:



Note Depending on whether you have a digital camera, the image may contain a lighter rectangular area. See "Calibrating the video image" for more information. ▲

   To make it easier to see details in the video image, you can enlarge the window by dragging its sides or corners.

6. **With the ATR crystal in the beam path, carefully make contact with the soot.**

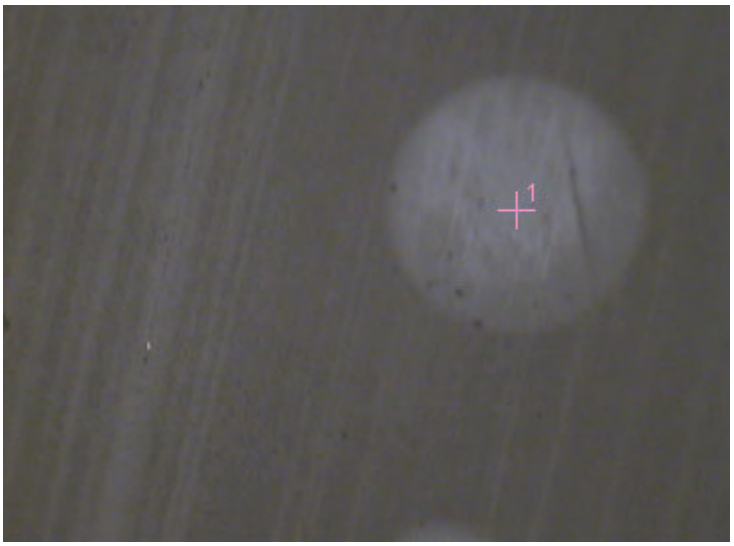
   If you have the internal Contact Alert System, use the ATR Contact button to make contact.

7. **Raise the objective and then, with the ATR crystal out of the beam path, refocus on the soot.**

   In the video image you will see a round, lightened area where the crystal made contact with the soot. Here is an example showing that the crystal is not centered on the field of view, indicating that calibration is needed:

8. **Drag the marker labeled "1" to the center of the round area.**

   You can use the buttons in the Refine Marker Position box to more finely adjust the position of the marker. Here is our example with the marker centered in the round area:



9. **Type a brief description of the calibration in the Brief Description text box.**

   This description will be listed in the Brief Description drop-down list box in the Select ATR Calibration dialog box after you save the calibration.

10. **Type a more detailed description of the calibration in the Full Description text box.**

    The full description is a good way to record what the calibration was created for. It's helpful to include a description of the objective that was used for the calibration.

    After you save the calibration, the full description will appear in the Select ATR Calibration dialog box when you select the calibration from the Brief Description drop-down list box.

11. **Click the Save button.**

    The saved calibration is now available for use. For more information see "Opening a saved ATR calibration."

12. **If you want to use the new calibration immediately, select it from the Brief Description drop-down list box and then click the Set Current button. When you are finished, click the Close button. Then close the System Configuration dialog box by clicking the OK button.**

    With the new calibration in effect, you can verify that it is working properly in the Atlμs window:

    a. With the ATR crystal out of the beam path, move the stage so that an unused area of soot fills the field of view and focus on the soot.

    b. With the ATR crystal in the beam path, carefully make contact with the soot.

c. Raise the objective and then, with the ATR crystal out of the beam path, refocus on the soot. The round, lightened area should be centered on the cross hairs in the video pane.

Note Before using the crystal for data collection, be sure to clean it by following the cleaning practices explained in the documentation that came with the objective or microscope. ▲

Opening a saved ATR calibration

Follow these steps to open a saved ATR calibration:

1. **Select the ATR calibration to open from the Brief Description drop-down list box in the Select ATR Configuration dialog box.**

   Information about the selected ATR calibration appears below the drop-down list box. This information was entered when the calibration was created (see "Performing an ATR calibration").

2. **Click the Set Current button.**

   The ATR calibration will be in effect when you next use the Atlμs window.

Deleting a saved ATR calibration

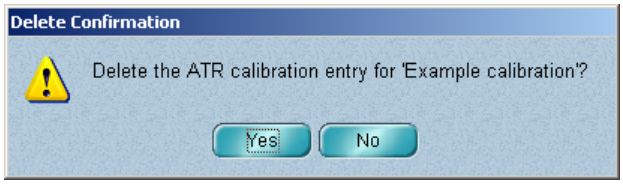
Follow these steps to delete a saved ATR calibration:

1. **Select the ATR calibration you want to delete from the Brief Description drop-down list box in the Select ATR Configuration dialog box.**

   Information about the selected ATR calibration appears below the drop-down list box. This information was entered when the calibration was created (see "Performing an ATR calibration").

2. **Click the Delete button.**

   A confirmation message appears. Here is an example:



3. **Choose Yes.**

Aligning the video cross hairs

It is possible for the video image cross hairs to become no longer aligned with the center of the microscope field of view (as defined by the eyepiece cross hairs). If this happens, you may notice that the position of a sample feature displayed in the video image does not exactly match its position as seen through the microscope viewer.

Follow these to use the Align Cross Hairs button to realign the video cross hairs:

1. **Place a sample on the stage and position a small sample feature at the center of the eyepiece cross hairs.**

   If the video cross hairs need alignment, the sample feature will not be centered on the cross hairs in the video pane of the Atlμs window. If the feature is centered, you do not need to align the cross hairs.

2. **Click the Align Cross Hairs button.**

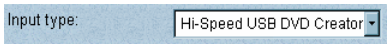
   A dialog box appears:

3. **Click the arrow buttons as needed to position the sample feature at the center of the video image cross hairs.**

   The arrows indicate the direction of movement. The X and Y values show how far the sample has moved, in micrometers.

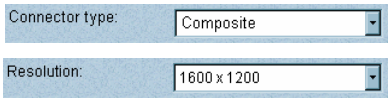
4. **When you are finished, choose OK.**

Specifying the video input type



Right after your system has been installed, select the type of frame grabber or digital camera you are using from the Input Type drop-down list box in the System Configuration dialog box. If you select a digital camera, specify its resolution as explained in the next section.

Specifying the video connector type or camera resolution



Right after your system has been installed, use Connector Type or Resolution in the System Configuration dialog box to select the type of video connector you are using or the camera resolution. The available parameter and its allowed settings depend on the setting of Input Type (see the preceding section).

Note If you are using a digital camera and notice slow operation of the software, try using a lower Resolution setting. If you later need to capture high-resolution images, you can temporarily use a higher Resolution setting for that purpose. ▲

Microscope configuration

Use the features in the Microscope box in the System Configuration dialog box to do the following:

- Select a microscope configuration.
- Initialize the stage.
- Initialize the automated Reflex aperture, if present.
- Limit the stage travel.
- Configure the microscope.

The next sections explain how to perform these tasks.

Selecting a microscope configuration

If your system has more than one microscope mapping product—for example, a Continuμm microscope and an FT-Raman View Stage—you need to specify the one to use for your next data collection. Simply select the appropriate option from the Current Configuration drop-down list box.

If you have a Nicolet Almega system, specify the microscope configuration by selecting Almega.

Initializing the stage

The following sections explain how to initialize the stage on FT-IR, FT-Raman and visible Raman systems.

Initializing the stage on an FT-IR or FT-Raman system

Use the X-Y Stage and Z-Axis buttons in the System Configuration dialog box to initialize the microscope stage within the horizontal plane (in the X and Y dimensions) and vertically (along the Z-axis), respectively.

Perform an X-Y initialization once right after the system is installed and any time you have moved the stage by hand when the stage power is off. You can also perform an X-Y initialization whenever you want to reset the origin (0,0) to the physical center of travel.

If you have a Continuμm microscope, perform a Z-axis initialization every time you turn on the microscope power.

Important Before initializing the stage, make sure it will not hit the objective, condenser, microscope body or anything else. If you have the XL motorized stage, make sure it is somewhere near the physical center of travel rather than close to its limit of travel. If the XL stage produces a grinding sound during initialization, turn off the controller, wait for the software to display an error message, turn on the stage power, center the stage and then restart initialization. ▲

To perform an initialization, click the appropriate button and then follow the instructions that appear on the screen.

Note The Z-axis button is not available if the microscope does not have a motorized Z-axis, the Z-axis does not require initialization, or the Z-axis has already been initialized an does not need to be reinitialized. If you have a Continuµm microscope and need to initialize the Z-axis but the button is not available, turn the microscope power off and then on and restart OMNIC Atlµs to make the button available. ▲

Initializing the stage on a visible Raman system

Use the X-Y Stage button in the System Configuration dialog box to initialize the microscope stage within the horizontal plane (in the X and Y dimensions). Perform an initialization once right after the system is installed and any time you have moved the stage by hand when the stage power is off. You can also perform an initialization whenever you want to reset the origin (0,0) to the physical center of travel.

To perform an initialization, click the button and then follow the instructions that appear on the screen.

Initializing the automated Reflex aperture

If your microscope has an automated Reflex aperture, you should adjust its size and shape by using any of these software features: the box that represents the Reflex aperture in the video pane of the Atlµs window, Set Aperture To Default in the Atlµs menu, Aperture Dimensions in the Atlµs menu, and the Aperture button on the Mapping tab of the Experiment Setup dialog box.

You should *not* also use a knob on the Continuμm microscope to adjust the aperture, because doing so can cause aperture misalignment. If this happens, click the Aperture button to initialize the aperture, returning it to correct alignment.

For information about adjusting the aperture, see "Adjusting the automated Reflex aperture graphically," "Setting the automated Reflex aperture numerically" and "Setting the automated Reflex aperture to the default" in the "Preparing for Data Collection" chapter.

Limiting the stage travel

Use the Limit Stage Travel button to limit the distance in the X and Y directions that the stage may travel. This is useful when the sample is small and you want to avoid accidentally setting up a map outside the area of the sample. By limiting the stage travel, you also define the limits of the navigation pane of the Atlμs window: If you zoom the pane all the way out, the zoom will go only as far as the defined limit. Restricting the travel range is also useful for ATR mapping.

Follow these steps:

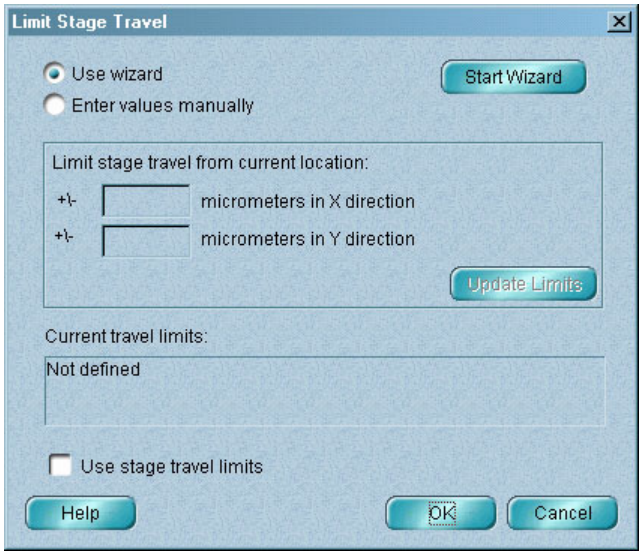
1. **If you want to specify the travel limits by typing distance values, move the stage to the location from which you want to specify the maximum distances.**

   The travel distance limits you specify will be relative to this location.

   If you want to specify the limits by moving the stage, you can start the procedure with the stage in any location.

2. **Click the Limit Stage Travel button in the System Configuration dialog box.**

   The Limit Stage Travel dialog box appears:



   The current travel limits, if defined, appear in the Current Travel Limits box.

3. **If you want to specify the travel limits by moving the stage to the limits, select Use Wizard and go to the next step. If you want to specify the limits by typing values, select Type Values and go to step 5.**

4. **Click the Start Wizard button.**

   The wizard guides you through specifying opposite corners of the desired range of stage travel. Follow the instructions that appear on the screen. When you are finished, the new limits appear in the Current Travel Limits box. Go to step 8.

5. **Type the desired maximum X travel distance, in micrometers, in the first text box.**

   The stage will not be able to move farther than this distance from the current stage location in either direction along the X-axis.

6. **Type the desired maximum Y travel distance, in micrometers, in the second text box.**

   The stage will not be able to move farther than this distance from the current stage location in either direction along the Y-axis.

7. **Click the Update Limits button.**

   The new limits appear in the Current Travel Limits box.

8. **If you want to use the specified limits immediately, select Use Stage Travel Limits.**

   If Use Stage Travel Limits is not selected, your settings will be saved, but not immediately used, when you choose OK. You will be able to select this option later to put the settings into effect. This lets you easily limit the stage travel just when you want to.

9. **Choose OK.**

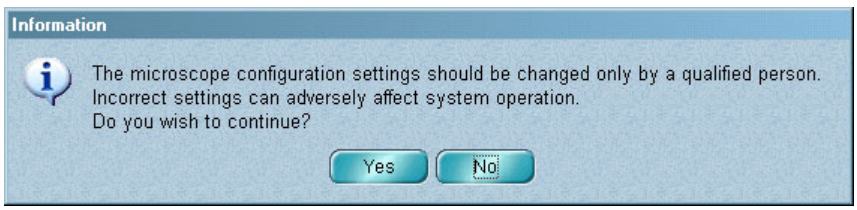
   When your stage travel limits are in effect, this icon appears near the upper-left corner of the Atlμs window:

Configuring the microscope

Right after your system has been installed, follow the general steps below to configure the microscope hardware with the Configuration button. The next sections explain the individual parameters in detail.

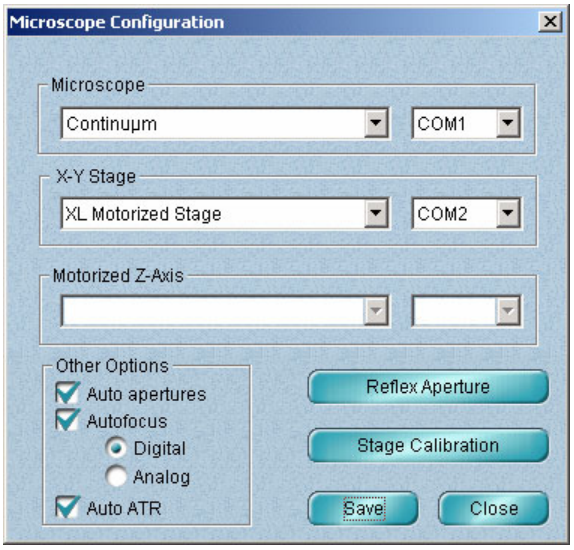
1. **Click the Configuration button in the System Configuration dialog box.**

   A message appears:



2. **Choose Yes if you are qualified to configure the microscope hardware. Choose No if you are not.**

   If you choose Yes, the Microscope Configuration dialog box appears:



A COM2 setting designates a USB port.

3. **Set the parameters as desired.**

4. **Choose Save.**

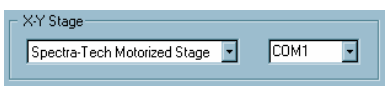
5. **Choose Close.**

   The saved settings will be in effect when you close the dialog box and when you later start OMNIC Atlμs.

Specifying the microscope model

Specify your microscope model by selecting the appropriate setting from the first drop-down list box in the Microscope box. If the drop-down list box to the right is available, use it to select the COM port you are using for the microscope.

Specifying the stage model



Specify your stage model by selecting the appropriate setting from the first drop-down list box in the X-Y stage box. Then select the COM port you are using for the stage from the drop-down list box to the right.

If you select XL Motorized Stage or Prior ProScan Motorized Stage, the Stage Calibration button becomes available. See “Calibrating the stage” for more information.

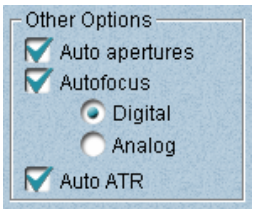
Specifying the motorized Z-axis

Specify the type of motorized Z-axis you are using by selecting the appropriate setting from the first drop-down list box in the Motorized Z-Axis box. Then select the COM port you are using for the hardware from the drop-down list box to the right, if it is available.

Note

Since the motorized Z-axis is an integral component of automated Continuμm microscopes, the Motorized Z-Axis parameters are not used for those microscopes. ▲

Setting the Auto Apertures, Autofocus and Auto ATR options



Select the appropriate options in the Other Options box to specify whether you have various hardware options:

If you have an automated Reflex aperture, select Auto Apertures to display the box representing the aperture in the video pane of the Atlμs window. The aperture tool is not available when this option is selected. See “Adjusting the automated Reflex aperture graphically” in the “Preparing for Data Collection” chapter for instructions for adjusting the aperture.

If you have the autofocus hardware, select Autofocus to display the Autofocus button in the Atlμs window. On some systems this automatically selects the appropriate autofocus option—Digital or Analog—and you cannot change the setting. On other systems you must select an option: If your microscope has a digital camera and the necessary electronics, select Digital. If you have an analog camera and the necessary electronics, select Digital only if you want to use the digital autofocus feature; otherwise, select Analog. The Digital option enables the digital autofocus feature, which requires calibration before first use; see “Autofocus calibration” in the “Preparing for data collection” chapter for instructions. (When you use the Autofocus button the first time, a message informs you if calibration is required.) See “Using the focus buttons” in the “Preparing for Data Collection” chapter for more information about using the Autofocus button.

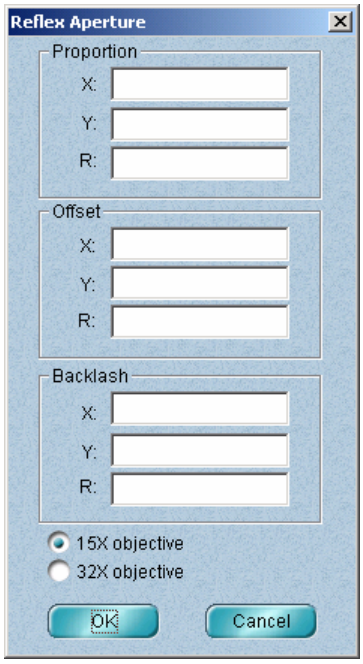
If you have the hardware needed for automated ATR contact, select Auto ATR to display the ATR contact button in the Atlμs window. See “Using the focus buttons” in the “Preparing for Data Collection” chapter for more information.

Calibrating the Reflex aperture

Right after your system has been installed, use the Reflex Aperture button once to calibrate the motion of the automated Reflex aperture, if present. Follow these steps:

1. **Click the Reflex Aperture button in the Microscope Configuration dialog box.**

   The Reflex Aperture dialog box appears:



2. **Type the appropriate values in the text boxes.**

   You can find the values on a label on the inside surface of the panel just below the microscope viewer. Use a screwdriver to remove the two screws that fasten the panel to the microscope. Replace the panel when you are finished entering the values.

3. **Specify the objective you are using by selecting the appropriate option near the bottom of the dialog box.**

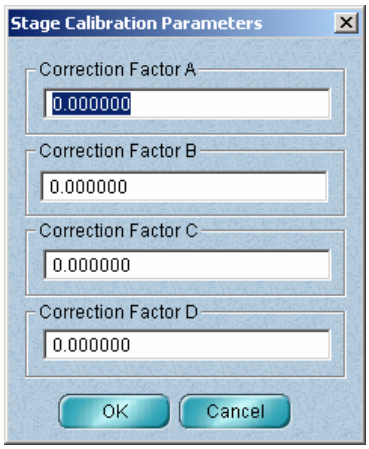
4. **Choose OK.**

Calibrating the stage

If you set X-Y Stage to XL Motorized Stage or Prior ProScan Motorized Stage, the Stage Calibration button becomes available. It lets you enter values to compensate for skewed stage movement that may result from mechanical tolerances. Do this once right after your system is installed. Follow these steps:

1. **Click the Stage Calibration button.**

   The Stage Calibration Parameters dialog box appears:



2. **Type the appropriate values in the text boxes.**

   You can find the values on a label on the bottom of the stage.

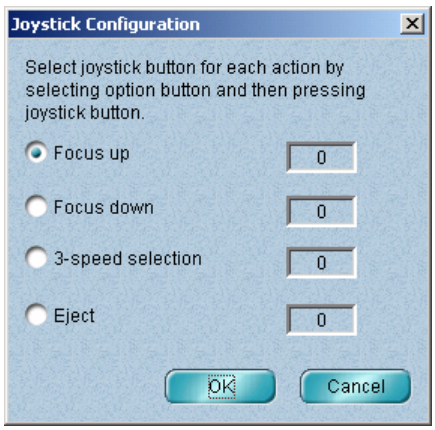
3. **Choose OK.**

Configuring the joystick

If you set Microscope to a Raman product that uses a joystick, the Joystick Configuration button becomes available. It lets you assign the actions that the joystick buttons perform. Follow these steps:

1. **Click the Joystick Configuration button.**

   The Joystick Configuration dialog box appears:



2. **Select an action to assign.**

   For example, if you want a button on the joystick device to move the stage upward for focusing, select Focus Up. The 3-Speed Selection option controls the speed of stage movement. The Eject option positions the stage for easiest removal of samples.

3. **Press the button on the joystick device that you want to use to perform the selected action.**

   The identification number of the button automatically appears to the right of the option.

4. **Repeat steps 2 and 3 for the other actions you want to assign.**

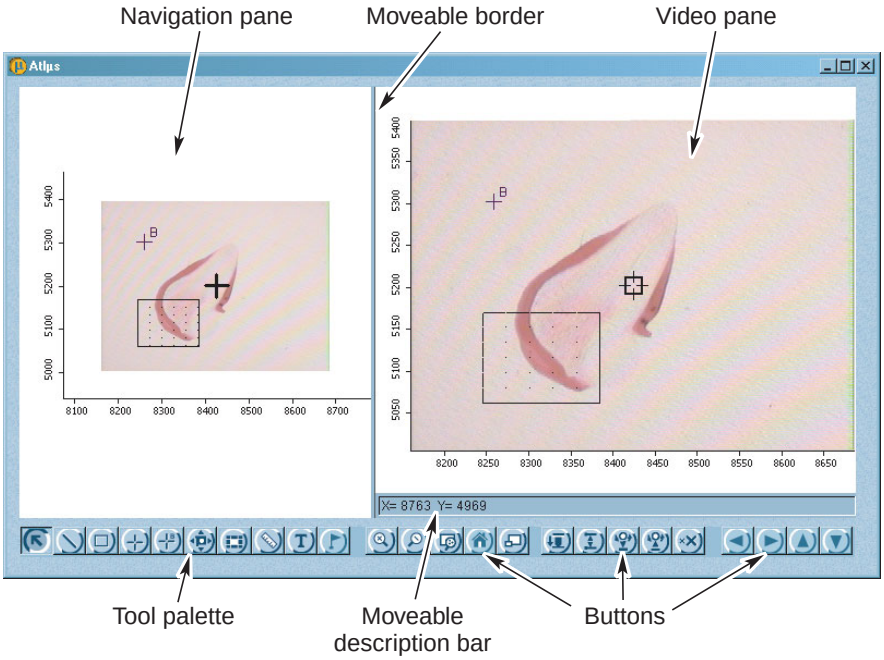
5. **Choose OK.**

Preparing for Data Collection

This chapter describes the Atlμs window and explains how to specify a map sequence and perform other operations to set up map data collection.

The Atlμs window

The Atlμs window provides features you need to set up a mapping experiment. The window appears when you choose Show Atlμs Window from the Atlμs menu.



Atlμs window

The Atlμs window contains two panes: the navigation pane and the video pane. These panes let you graphically specify a map sequence and view the sample. You can change the sizes of the panes by dragging the border that separates them to the left or right.

At the bottom of the Atlμs window are several tools and buttons you can use to draw maps and apertures (if available), adjust the display of information in the panes and perform other operations. These are described later in this chapter.

Note If you have a Continuμm microscope with the automated Reflex aperture system, the aperture tool does not appear in the window; you use other features to specify the size and orientation of the aperture. See "Setting the automated Reflex aperture" for details. If your microscope does not have this feature, the aperture tool is provided. ▲

The description bar displays information about the operation you are performing or tool you are currently using. You can drag the description bar from the bottom of one pane to the other according to your preferences.

The navigation pane

The navigation pane of the Atlμs window shows graphically the possible range of movement of the microscope stage. The X-axis and Y-axis of the pane correspond to the side-to-side and front-to-back movements of the stage, respectively. You can change the displayed stage area by using the palette tools and the buttons near the bottom of the window. These are explained later in this chapter.

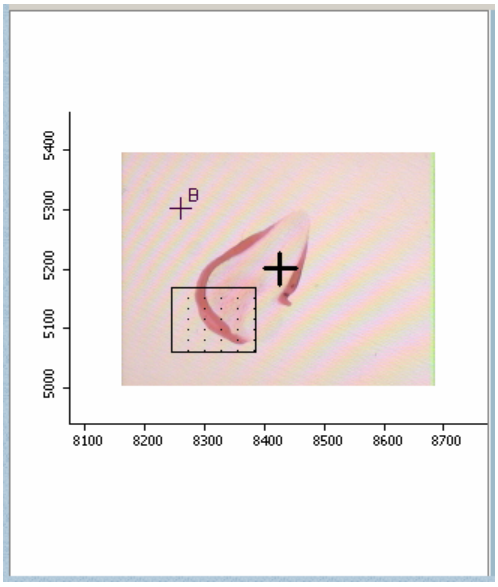
If you display the entire range of movement in the navigation pane, the video image is too small to be seen.

The navigation pane includes a video image of the sample area being viewed. This image is a copy of the live video image displayed in the video pane, although it may be larger or smaller depending on how you have adjusted the display. The copy is updated whenever the stage moves or the navigation pane is resized or moved.

Here is an example showing the navigation pane with an area map drawn and a background point (labeled “B”) specified:

A copy of the video image appears in the pane, although it may be too small to be seen. In this example it has been enlarged by zooming in.

The cross hairs indicate the center of the current field of view.



Navigation pane

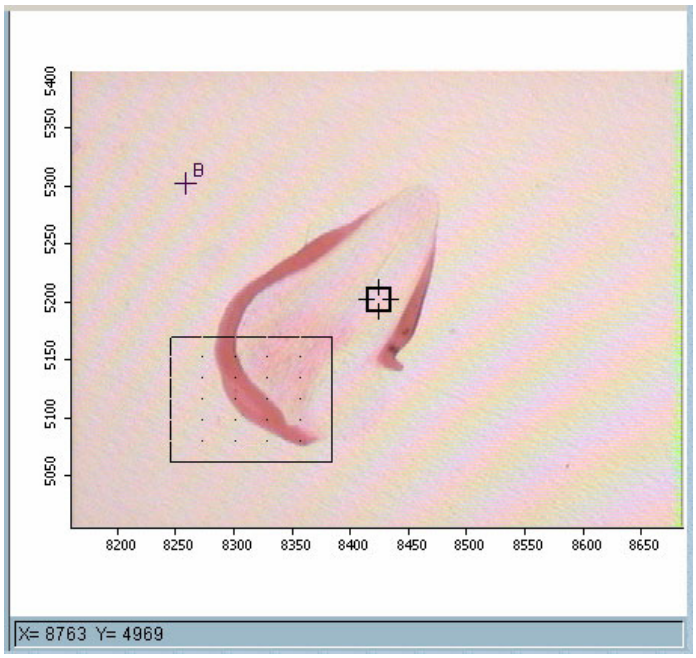
You can use the Atlμs window tools within the navigation pane to specify the size and location of a map and the location of the background point, if appropriate. See “The tool palette” for more information.

The X and Y proportions (aspect ratio) of the navigation pane always match those of the video pane, except when you use the Full Range View button in the Atlμs window to show the entire range of stage movement. Because of this, any map you draw in a zoomed-in area of the navigation pane will have the same shape in the video pane. Together, the matching proportions and the copy of the video image make it easy to see the correspondence between the two panes as you change the view of the sample.

The video pane

The video pane at the right side of the Atlμs window displays a live video image of the sample surface. The stage coordinates that are visible within the pane are indicated by the X-axis and Y-axis.

Here is an example showing the video pane with an area map drawn and a background point (labeled “B”) specified:



The “target” cross hairs indicate the center of the field of view.

Video pane

You can display different areas of the sample in the video pane by using the stage movement tool (see “Moving the stage by clicking a point”) or the stage movement buttons (see “Changing the view with the stage movement buttons”).

You can use the Atlμs window tools within the video pane to specify the size and location of a map and the location of the background point, if appropriate. See “The tool palette” for more information.

Because the X and Y proportions (aspect ratio) of the navigation pane always match those of the video pane (except when you use the Full Range View button in the Atlμs window to show the entire range of stage movement), any map you draw in the video pane will have the same shape in a zoomed-in area of the navigation pane.

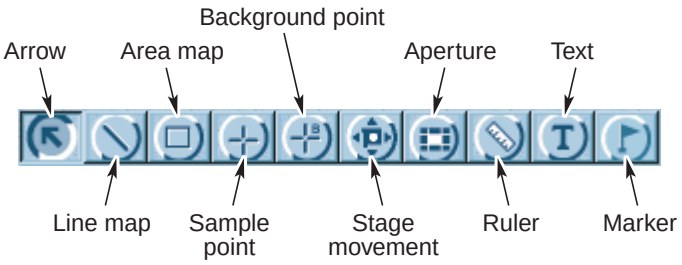
You can copy the video image to the Windows Clipboard by choosing Copy Video Image from the Edit menu. You can then paste the image into a document using a word processing program or other program that lets you paste items from the Clipboard.

If you have a Continuµm microscope with the automated Reflex aperture system (must be installed by Thermo Electron), the Reflex aperture is represented in the video pane by a box whose size, shape and orientation you can manipulate. This manipulation adjusts the aperture in the microscope. See “Adjusting the automated Reflex aperture graphically” for instructions.

The tool palette

The tool palette provides you with tools for graphically specifying and manipulating map sequence information in the Atlµs window.

The provided tools depend on your system. A red line may appear on a tool if it cannot be used under the current conditions (for example, when a Z-axis initialization needs to be performed).



When you move a tool’s pointer into the navigation pane or video pane, the coordinate values of the pointer location appear in the description bar. Also, the appearance of the pointer may change to indicate which tool is selected.

The table below shows what you can do with each tool:

Tool		Uses
	arrow tool	Adjust the automated Reflex aperture, if available. (See “Adjusting the automated Reflex aperture graphically” for details.) Move the stage or a sample point, background point (if available), line map, area map, ruler, text annotation, marker or box drawn to specify a Mosaic. Briefly move the stage to every sample and background point (if available) in order (Check Points command). Resize a line map, area map, drawn aperture (if available), ruler, or box drawn to specify a Mosaic. Delete a map, sample point, background point (if available), aperture (if available), ruler, text annotation or marker.

Tool		Uses
		Clear a map sequence. Edit text annotation. Move the stage by dragging the cross hairs. Rotate a drawn aperture (if available). Set the video source parameters. Set home to the current stage location.
	line map tool	Draw a line map. Move a line map. Resize a line map. Add a background point (if available). Delete a line map. Set the video source parameters.
	area map tool	Draw an area map. Move an area map. Resize an area map. Add an ordered array of discrete points. Add a background point (if available). Delete an area map. Set the video source parameters.
	sample point tool	Add a sample point or background point (if available). Move a sample point, background point (if available) or marker. Move the stage to a sample point. Delete a sample point. Specify whether to capture the video image for a sample point (Toggle Capture Video For Sample Point command). Set the video source parameters. Set the Z (vertical) position of a sample point to the current Z position.

Tool		Uses
	background point tool (if available)	Add a background point. Move a background point, sample point or marker. Move the stage to the background point. Delete a background point. Set the video source parameters.
	stage movement tool	Move the stage to a point. Set the video source parameters.
	aperture tool (if available)	Draw an aperture. Resize a drawn aperture. Delete a drawn aperture. Set the drawn aperture to its default size and zero degrees of rotation. Set the video source parameters.
	ruler tool	Draw a ruler. Move a ruler. Resize a ruler. Set the video source parameters.
	text tool	Add text annotation. Edit text annotation. Delete text annotation. Set the video source parameters.
	marker tool	Add a marker. Move a marker, sample point or background point (if available). Move the stage to a marker. Delete a marker. Delete all the displayed markers. Set the video source parameters.

All of these operations, except setting the video source parameters, are explained later in this chapter. See “Setting the video source parameters” in the “Configuring the System” chapter for information about setting the video source parameters.

Changing the view by moving the stage

There are several ways to change your view of a sample by moving the stage. These are explained in the next sections.

Changing the view with the stage movement buttons

The stage movement buttons let you move the stage in four directions. The distance the stage moves when you click a button depends on the dimensions of the video field of view and the direction of movement. Each time you click a button, the stage moves one full video frame. The video pane axes change to reflect the new stage coordinates represented by the pane.

Click this button to see a portion of the sample that is to the left of the displayed video frame. The stage X coordinates decrease.

Click this button to see a portion of the sample that is to the right of the displayed video frame. The stage X coordinates increase.

Click this button to see a portion of the sample that is “above” the displayed video frame. The stage Y coordinates increase.

Click this button to see a portion of the sample that is “below” the displayed video frame. The stage Y coordinates decrease.

Moving the stage by clicking a point

Follow the steps below to quickly move the stage to position a specified point under the microscope objective. The point becomes the center of the video image in the video pane.

1. **Select the stage movement tool.**

2. **Click the point in the navigation pane or video pane that you want positioned under the microscope objective.**

   When you click the point, the stage moves as needed to position the point under the objective. The video image is redisplayed with the point at the center, and the video pane axes are adjusted accordingly. The clicked point is also marked with cross hairs in the navigation pane.

Note The stage movement tool is useful for verifying that the video image is calibrated and that the X and Y axes are set correctly. Use the tool to click a location in the video pane. If that location moves to the center of the video pane, the calibration and settings are correct. ▲

Moving the stage by dragging the cross hairs

You can use the arrow tool to move the stage. Follow these steps:

1. **Select the arrow tool.**

2. **Drag the cross hairs in the navigation pane or video pane to the desired location.**

   When you release the mouse button, the stage moves and the panes' axis labels are updated to reflect the new position.

Moving the stage to its home position

Click the Move Stage To Home button to move the stage horizontally to the location defined as "home" (the location whose coordinates are 0,0). You can set home to the current stage location by *right-clicking* the navigation pane or video pane with the arrow tool and choosing Set Home To Current from the pop-up menu. You can set home to the current stage location or to its original location by using the Move Stage command in the Atlμs menu. See "Moving the stage with the Move Stage command" for details.

Moving the stage to the origin point

Choose Go To Origin from the Atlμs menu to move the stage to the origin point (the "home" location, whose coordinates are 0,0).

Moving the stage to a sample point

Follow these steps to move the stage to a sample point you have specified with the sample point tool (see "Specifying discrete sample points"):

1. **Select the sample point tool.**
2. ***Right-click* the sample point.**
3. **Choose Move To Point from the pop-up menu.**

Moving the stage to a background point

Follow these steps to move the stage to a background point you have specified with the background point tool, if available (see "Specifying a background point"):

1. **Select the background point tool or sample point tool.**
2. **If you selected the background point tool, *right-click* anywhere in the navigation pane or video pane. If you selected the sample point tool, *right-click* the background point.**
3. **Choose Move To Background Point or Move To Point from the pop-up menu.**

Moving the stage to every sample and background point

Follow the steps below to briefly move the stage to every sample point and background point (if available) in order. This lets you review the sequence of points that will be used in the map collection.

1. **Select the arrow tool.**
2. ***Right-click* anywhere in the navigation pane or video pane.**
3. **Choose Check Points from the pop-up menu.**

   The stage starts to move to the points. You can cancel the operation by pressing the Esc key on the keyboard.

Moving the stage to a marker

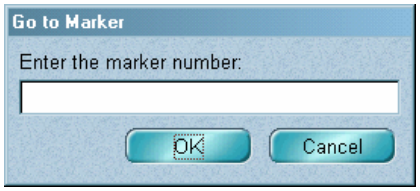
Follow these steps to move the stage to a marker you have added with the marker tool (see "Adding a marker"):

1. **Select the marker tool.**

2. ***Right-click* anywhere in the navigation pane or video pane.**

3. **Choose Move To Marker from the pop-up menu.**

   The Go To Marker dialog box appears:



4. **Type the number of the marker.**

   You can type the number with or without the "M" in front of it.

5. **Choose OK.**

   The stage moves to the marker. You can cancel the operation by pressing the Esc key on the keyboard.

Moving the stage with the Move Stage command

Use Move Stage in the Atlμs menu to move the stage in any of these ways:

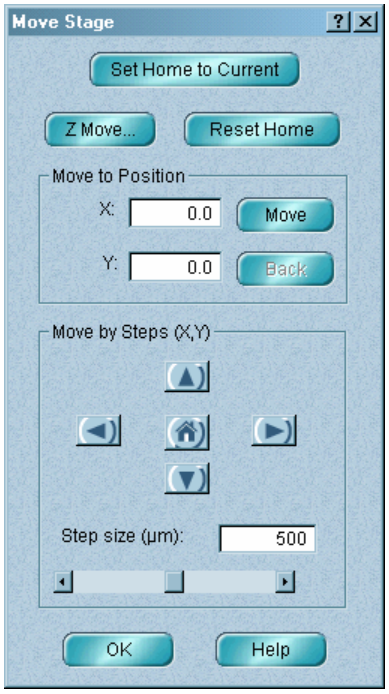
- In one operation to a point whose coordinates you specify.
- Incrementally along the X-axis or Y-axis.
- Along the Z-axis.

You can also set the current X-Y position as the "home" position (the location whose coordinates are 0,0) or reset the home position to its original location. See "Moving the stage to its home position" for information about moving the stage to this position later.

Follow these steps:

1. **Choose Move Stage from the Atlµs menu.**

   The Move Stage dialog box appears showing the current X and Y stage coordinates in the Move To Position box:



2. **Move the stage as desired.**

   - To move the stage to a numerically specified point, type the desired X and Y coordinates in the X and Y text boxes in the Move To Position box, and then click the Move button. The stage moves to the specified point. To return the stage to its previous position, click the Back button.

   - To move the stage a specified distance along its X-axis or Y-axis, first type the desired distance in micrometers in the Step Size (µm) text box in the Move By Steps (X,Y) box or use the scroll bar to change the value. Then click the button labeled with the desired direction of movement.

The table below explains how the buttons move the stage.

This button…	Does this…
	Moves the stage to the right to display a portion of the sample that is to the left of the current video frame. The stage X coordinate decreases.
	Moves the stage to the left to display a portion of the sample that is to the right of the current video frame. The stage X coordinate increases.
	Moves the stage toward the front to display a portion of the sample that is “above” the current video frame. The stage Y coordinate increases.
	Moves the stage toward the rear to display a portion of the sample that is “below” the current video frame. The stage Y coordinate decreases.

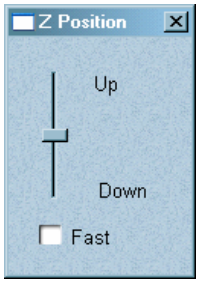
Each time you click a button, the stage moves the specified distance in the indicated direction. This lets you move the stage incrementally toward or away from a sample feature.

Click this button if you want to move the stage to the location defined as “home” (the location whose coordinates are 0,0).

You can set home to the current stage location by clicking the Set Home To Current button. (You can also do this by *right-clicking* the navigation pane or video pane in the Atlμs window and choosing Set Home To Current from the pop-up menu.)

Click the Reset Home button to reset the home position to the location it had immediately after the stage was initialized (the center of the stage).

- To move the stage up or down along the Z-axis, click the Z Move button. The Z Position dialog box appears:



Important Be careful not to hit the objective with the sample or stage when moving the stage up. ▲

To move the stage up or down, drag the horizontal bar up or down, respectively, and hold it until the stage is in the desired vertical position. Then release the mouse button. If your mouse has a wheel, you can use it to control the bar and move the stage. You can also press the up and down arrow keys on the keyboard to move the stage vertically.

To increase the speed of the stage movement, select Fast, or hold down the Shift key while you drag the bar.

When you are finished, click the Close button (labeled "X"). The dialog box closes automatically after 5 seconds if you start using another feature.

3. When you are finished moving the stage, choose Close.

Zooming in or out

There are several ways to zoom in on an area in the navigation pane or zoom out. These are explained in the next sections.

Using the zoom buttons

The zoom buttons let you quickly zoom in on the area of the stage you are viewing in the navigation pane or zoom out from the stage to see a larger area.

Click the Zoom In button to decrease the area of the stage represented in the navigation pane. The cross hairs indicate the center of the area.

Click the Zoom Out button to increase the area of the stage represented in the navigation pane. The maximum size of the stage area represented by the pane is the maximum travel allowed by your stage controller.

Note You can limit the range of travel by using the Limit Stage Travel button in the System Configuration dialog box. See "Limiting the stage travel" in the "Configuring the System" chapter. ▲

Zooming in on a map

Click the Zoom To Points button in the Atlμs window to instantly zoom in on a map displayed in the navigation pane. This is useful if you have zoomed out from the map to view a larger stage area and the map is now displayed too small to be seen clearly.

Displaying the full range of stage travel

Click the Full Range View button to zoom all the way out to display the full range of stage travel allowed by your stage controller.

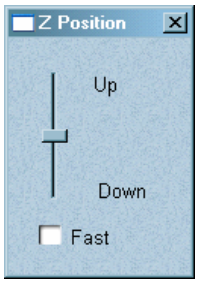
Note You can limit the range of travel by using the Limit Stage Travel button in the System Configuration dialog box. See "Limiting the stage travel" in the "Configuring the System" chapter. ▲

Using the focus buttons

If you have the required hardware, you can use the focus buttons to focus the microscope:

Click the ATR Contact button (if available) to automatically move the stage upward to make optimal contact with an ATR sample. After contact is made, you can click the button to release contact. See "Using auto ATR contact" in the "Collecting Map Data" chapter for complete information.

Click the Z Position button to display a dialog box that lets you move the stage up or down:



Important Be careful not to hit the objective with the sample or stage when moving the stage up. ▲

To move the stage up or down, drag the horizontal bar up or down, respectively, and hold it until the stage is in the desired vertical position. Then release the mouse button. If your mouse has a wheel, you can use it to control the bar and move the stage. You can also press the up and down arrow keys on the keyboard to move the stage vertically.

To increase the speed of the stage movement, select Fast, or hold down the Shift key while you drag the bar.

When you are finished, click the Close button (labeled "X").

If you click the Autofocus button (requires the optional autofocus hardware), the system focuses on the sample automatically by moving the stage up or down. See "Autofocus calibration" for information about calibrating digital autofocus.

Click the Store Z Position button to save the Z (vertical axis) coordinate of the current stage position so that you can return to it later with the Recall Z Position button.

Click the Recall Z Position button to move the stage to the Z coordinate that was last saved with the Store Z Position button. The Recall Z Position button is available only if the Store Z Position button has been used to save the Z coordinate.

Autofocus calibration

If your system has digital autofocus and Digital is selected in the Microscope Configuration dialog box, you must calibrate the digital autofocus the first time you use the Autofocus button. See "Setting the Auto Apertures, Autofocus and Auto ATR options" in the "Configuring the System" chapter for more information.

Follow these steps to perform an autofocus calibration:

1. **Place a high-contrast sample on the stage.**

   The provided soda can sample works well for this.

2. **Click the Autofocus button.**

   A prompt says that the digital autofocus must be calibrated.

Note If the prompt does not appear, the digital autofocus has already been calibrated or the system does not include the digital autofocus feature. Skip this procedure. ▲

3. **Choose OK.**

   A prompt appears.

4. **Focus on the sample surface and then choose OK.**

   A prompt appears.

5. **Adjust the vertical position of the stage so that the sample is no longer in focus, and then choose OK.**

   Do not change move the stage horizontally.

   A prompt appears.

6. **Turn off the illumination or adjust the view selector for viewing through the eyepieces only, and then choose OK.**

   A message says the calibration is complete.

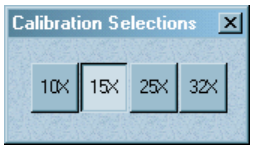
7. **Choose OK.**

Selecting a calibration

Use the Show Calibration Bar button to quickly select a saved calibration. Follow these steps:

1. **Click the Show Calibration Bar button.**

   A dialog box appears. Here is an example:



   Each calibration you have saved is represented by a button labeled with the magnification of the objective used to create the calibration. See "Calibrating the video image" in the "Configuring the System" chapter for more information.

2. **Click the button for the calibration you want to use.**

   If you are using an FT-Raman View Stage, click the Fixed button.

   The video pane changes to reflect the selected calibration.

3. **Close the dialog box by clicking its Close button (labeled "X" in the upper-right corner).**

Specifying a map sequence

To specify a map sequence for collecting a map, you can open a saved sequence or create a new sequence, as explained in the next sections.

Opening a map sequence

Map sequence settings are saved in experiment files. (See "Saving a map sequence" for more information.) To open a map sequence, open the experiment that contains it. You can do this by selecting an experiment from the Experiment drop-down list box below the menu bar or by using the Open button in the Experiment Setup dialog box (available through Experiment Setup in the Collect menu). Make sure the Map check box is selected in the Open Experiment dialog box. If you are using OMNIC, choose OMNIC Help Topics from the Help menu, find "Experiment Setup command" in the Index and go to the "Using Experiment Setup" topic for more information. If you are using OMNIC For Raman, choose Raman Help Topics from the Raman menu, find "Experiment Setup command" in the Index and go to the "Setting the experiment parameters" topic.

Note You can also use Open in the File menu to open a sequence file saved using an earlier version of OMNIC Atlμs. To allow you to locate and select a sequence file, set Files Of Type in the Open dialog box to Sequence Files (*.SEQ). Opening a sequence file has the same effect as opening a sequence that is part of an experiment. ▲

When you open a map sequence, the map it defines is displayed in the navigation pane. The map may also appear in the video pane depending on the stage coordinates currently represented by the pane.

The opened map sequence replaces any map sequence already displayed in the Atlμs window. If you want to save that sequence, be sure to do so before opening a map sequence.

Drawing maps and other items in the Atlμs window

You can use the palette tools to draw a map, sample points, an aperture (if available), a ruler and other items in the navigation and video panes. The next sections explain how.

Drawing a line map

Follow the steps below to draw a line map. The new map replaces any currently displayed map or sample points.

1. **Select the line map tool.**

2. **Point to the location in the navigation pane or video pane where you want the line to start.**

Note In most cases the starting and ending points of a line map are determined by the X values of both endpoints. The endpoint with the lower X value is designated the starting point; the endpoint with the greater X value is the ending point. Therefore, depending on how you draw the line, the point where you start drawing may be the starting or ending point when you are finished. If the X value is the same for all points, the starting point is the point with the lowest Y value. ▲

3. **Press and hold down the mouse button.**

4. **Move the pointer to the location where you want the line to end.**

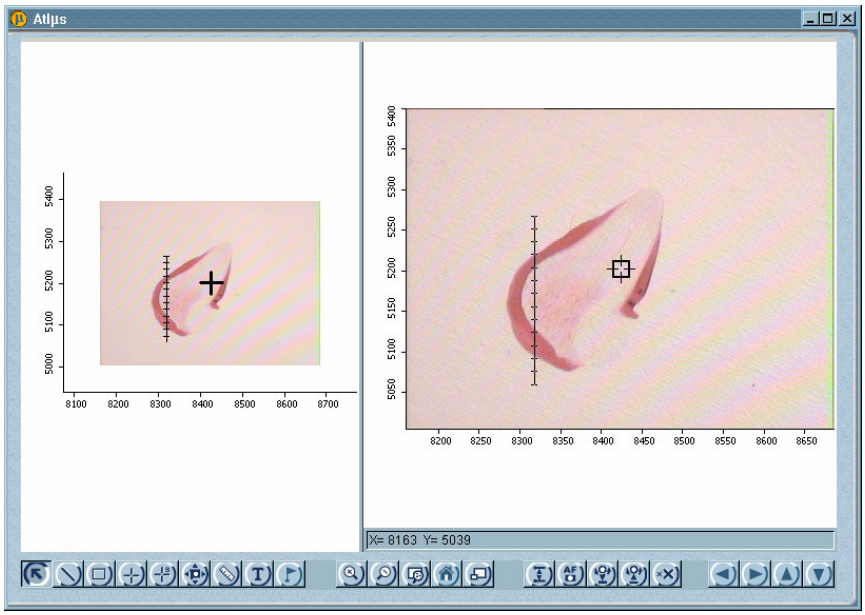
   The line changes in length and direction as you move the mouse.

5. **Release the mouse button.**

   If there was a map displayed in the pane, it is replaced by the new line map.

   When you draw a map in the navigation pane or video pane, the map appears in both panes, although you may need to zoom in to see the map in the navigation pane. See “Using the zoom buttons” for more information.

The following illustration shows a drawn line map in the navigation and video panes:



The tick marks on the line indicate the locations of sample points.

Note When you release the mouse button, the length of the map may vary from the line you drew by dragging. This is because the size of the map must be adjusted for the default step size specified on the Mapping tab in the Options dialog box (or to the aperture size default). “Specifying a default step size” for more information.

For example, if you used the mouse to specify a line map with a length of 100 micrometers and the step size is set to 22 micrometers, the length is automatically adjusted to 110 micrometers so that the step size is divided evenly into the map length. Map lengths always expand to compensate for step intervals; they are never less than the length you specified with the mouse. ▲

The next time you use Experiment Setup in the Collect menu, the information for the map will appear on the Mapping tab. You can specify a line map numerically by entering X and Y values on that tab. See “Setting the mapping parameters” for details.

To clear the map and start over, choose Clear Map Sequence from the Edit menu. See “Clearing a map sequence” for complete information.

Drawing an area map (or Mosaic)

Follow the steps below to draw an area map or specify a sample area for capturing a Mosaic of video images of that area. (See "Capturing a Mosaic of video images for a sample area" for more information.) The new map replaces any currently displayed map.

1. **Select the area map tool.**

2. **Point to the position in the navigation pane where you want a corner of the map (or Mosaic) to be located.**

   If you are drawing an area map rather than an area for capturing a Mosaic, you can draw the map in the video pane if desired.

3. **Press and hold down the mouse button.**

4. **Move the pointer to where you want the opposite corner of the map (or Mosaic) located.**

   The map (or box for specifying the Mosaic) changes size and shape as you move the mouse.

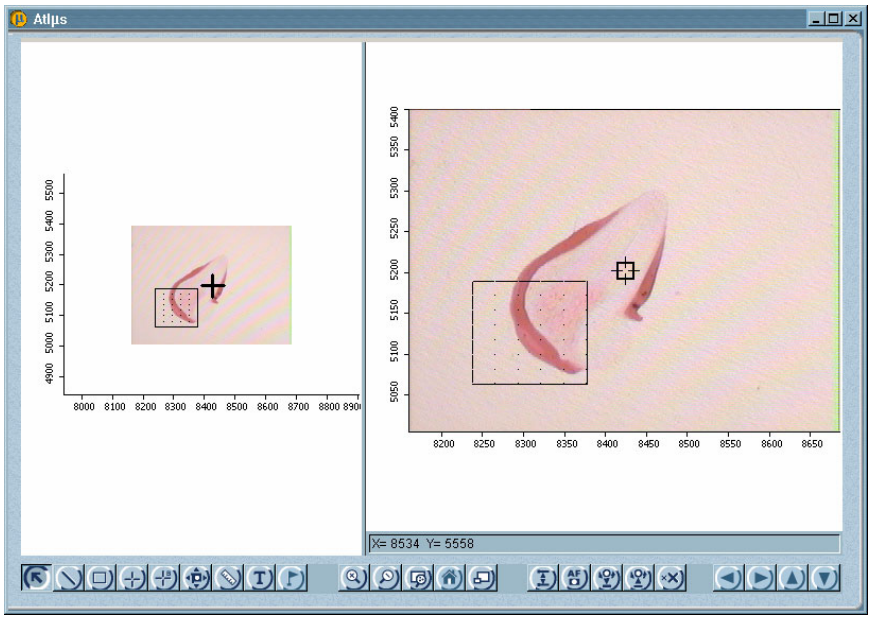
5. **Release the mouse button.**

   If there was a map displayed in the pane, it is replaced by the new area map (or box).

   When you draw a map in the navigation pane or video pane, the map appears in both panes, although you may need to zoom in to see the map in the navigation pane. (See "Using the zoom buttons" for more information.) In the video pane each sample point within the map is indicated by a dot. If the map is larger than the video pane, only the sample points within the limits of the pane will be visible.

If you have set Detector on the Bench tab of the Experiment Setup dialog box to XL Array (see "Specifying the detector for the Continuμm XL"), the Y dimension of the drawn area map (or box) "snaps" to the Y dimension of the linear array, or to a multiple of that dimension. This ensures that the full linear array is used when data is collected.

The following illustration shows a drawn area map in the navigation and video panes:



In the video pane the dots indicate the locations of sample points.

Note When you release the mouse button, the map may vary from the area you specified using the mouse. This is because the size of the map must be adjusted for the default step size specified on the Mapping tab in the Options dialog box (or to the aperture size default). "Specifying a default step size" for more information.

For example, if you used the mouse to specify a map area of 100 by 100 micrometers and the step size is set to 23 micrometers in both the X and Y dimensions, the map area is automatically adjusted to 115 by 115 micrometers so that the step size is divided evenly into the map area. Map areas always expand to compensate for step intervals; they are never less than the area you specified with the mouse. ▲

The next time you use Experiment Setup in the Collect menu, the information for the map will appear on the Mapping tab. You can specify an area map numerically by entering X and Y values on that tab. See “Setting the mapping parameters” for details.

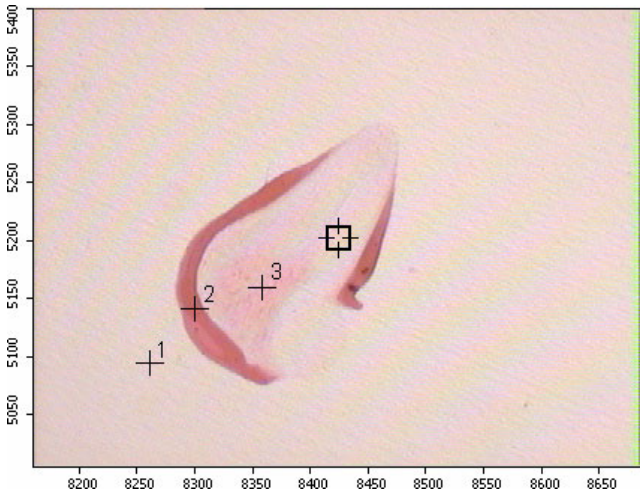
To clear the map (or box) and start over, choose Clear Map Sequence from the Edit menu. See “Clearing a map sequence” for complete information.

Specifying discrete sample points

You can use the sample point tool to specify individual locations, or “discrete points,” on the sample for collecting sample spectra. They replace any map that is currently displayed.

To add a sample point, click a location in the navigation pane or video pane. A consecutively numbered cross hairs marker appears. Here is an example:

The following illustration shows three discrete sample points specified in the video pane:



Note If you have the optional autofocus feature, you can focus the microscope before specifying each point. Each focus position (Z value) is stored and will be used by the Use Stored Focus Locations (Discrete Points Only) option in the Focus dialog box (available through Focus on the Mapping tab of the Experiment Setup dialog box). ▲

If a line map or area map is currently displayed, it is removed when you specify the first point.

When you specify points in the navigation pane or video pane, the points appear in both panes, although you may need to zoom in to see the points in the navigation pane. See "Using the zoom buttons" for more information.

You can move any point by using the arrow tool, as explained in "Moving a discrete sample point or background point."

To clear all the points and start over, choose Clear Map Sequence from the Edit menu. See "Clearing a map sequence" for complete information.

Using different aperture settings for discrete points

If you have a Continuμm microscope with the automated Reflex aperture, you can specify a different aperture size, shape and orientation for each point in a discrete-point collection. This is useful when the sample surface around the points of interest varies, and using a different aperture to isolate the desired area would improve the collected data. If you specify different aperture settings for the sample points, a new background is collected using the appropriate aperture setting for each point.

Follow these steps:

1. **Center the first sample area of interest in the video pane.**

2. **Adjust the Reflex aperture as desired for the first sample point.**

3. **Use the sample point tool to click the center of the cross hairs in the video pane.**

   This specifies the first sample point and stores the aperture settings in memory.

4. **Repeat the above steps for the next sample points.**

   Each time you specify a sample point, the aperture settings for that point are stored in memory.

5. **Specify the background location for the collection.**

   Whenever the aperture is adjusted for a sample point during collection, the system will automatically collect a new background at the background location using the new aperture setting.

6. **Choose Collect Map from the Collect menu to collect the spectra.**

   Before each spectrum is collected, the system automatically adjusts the aperture to the stored settings.

Specifying an ordered array of discrete points

If your samples are regularly spaced on a microscope slide or other suitable surface, you can use the area map tool to specify an "ordered array" of discrete points that matches the sample locations. The points replace any map that is currently displayed. Follow these steps:

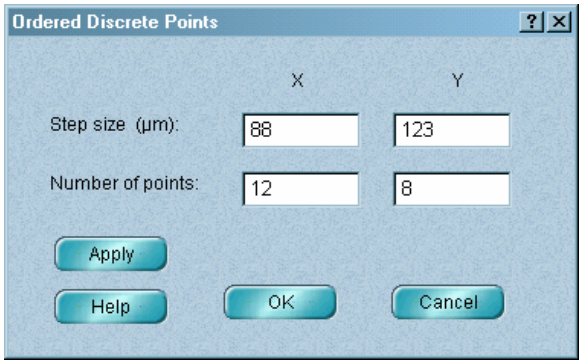
1. **Select the area map tool.**

2. **Draw a rectangle in the navigation pane or video pane to specify the area in which you want the ordered array located.**

3. ***Right-click* anywhere in the navigation pane or video pane.**

4. **Choose Ordered Discrete Points from the pop-up menu.**

   The Ordered Discrete Points dialog box appears:

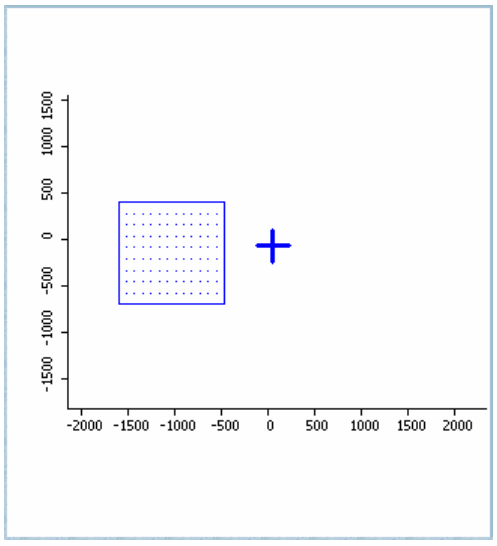


5. **Type the desired step sizes and number of points in the text boxes.**

6. **If you want to see the results of your settings in the Atlµs window before closing the dialog box, click the Apply button.**

7. **When you are finished, choose OK.**

   Here is an example of an ordered array in the navigation pane:



Note You can use the *right* mouse button to click a location in the navigation pane or video pane for the background point (if available) for the map. A cross hairs marker with the letter "B" appears, replacing any previously specified background point. The next time you use Experiment Setup in the Collect menu, the information for the specified background point will appear on the Mapping tab. See "Setting the mapping parameters" for details. ▲

To clear all the points and start over, choose Clear Map Sequence from the Edit menu. See "Clearing a map sequence" for complete information.

Setting the Z position for a discrete point to the current Z position

Follow the steps below to set the Z (vertical) position for a discrete sample point to the current Z position with the sample point tool. If Use Stored Focus Locations (Discrete Points Only) is selected in the Focus dialog box (available through the Focus button on the Mapping tab of the Experiment Setup dialog box), the stage will automatically move to the set Z position before collecting data at that point. See "Setting the focus parameters" for more information.

1. **Select the sample point tool.**

2. ***Right-click* the sample point in the navigation pane or video pane.**

3. **Choose Set Z Position To Current from the pop-up menu.**

Specifying a background point

Follow the steps below to specify where on the sample to collect a background spectrum for an FT-IR map. The point replaces any background that is currently displayed.

1. **Select the background point tool.**

   You can also select the sample point tool, line map tool or area map tool.

2. **Click the location in the navigation pane or video pane where you want to collect a background.**

   If you are using the sample point tool, line map tool or area map tool, *right-click* the location and then choose Add Background Point from the pop-up menu that appears.

   A cross hairs marker with the letter "B" appears at the clicked location, replacing any previously specified background point.

   If you have a Continuμm XL microscope and have selected Use Linear Array Detector For Map Setup in the Collect dialog box (available through the Collect button on the Mapping tab of the Experiment Setup dialog box), a rectangular cursor is overlaid on the cross hairs in the navigation pane. Here is an example:

   This cursor shows the size and shape of the linear array, allowing you to position the background point so that the area of the linear array does not overlap the area where you will collect sample data. See "Setting special mapping options" in the "Preparing for Data Collection" chapter for more information.

   When you specify a background point in the navigation pane or video pane, the point appears in both panes, although you may need to use the Zoom In button to see the point in the navigation pane. See "Using the arrow tool to zoom in" or "Using the zoom buttons" for more information.

   You can move the background point by using the arrow tool, sample point tool, background point tool or marker tool, as explained in "Moving a discrete sample point or background point."

The next time you use Experiment Setup, the location of the background point will appear on the Mapping tab.

To clear the background point and all the sample points, choose Clear Map Sequence from the Edit menu. See "Clearing a map sequence" for complete information.

Drawing an aperture

Use the aperture tool (if available) to draw a rectangular aperture in the video pane. The drawn aperture is always centered about the cross hairs in the pane, which reflect the current stage position.

Note If you have a Continuμm microscope with the automated Reflex aperture system, the aperture tool is not needed and therefore not available. See "Setting the automated Reflex aperture" for information on adjusting the aperture. ▲

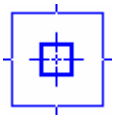
Follow these steps to draw an aperture:

1. **Install a rectangular aperture in the microscope and focus so that the aperture is clearly visible in the video pane.**

   If the aperture is adjustable, adjust its size and shape as desired.

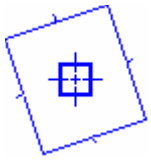
2. **Select the aperture tool.**

   A box representing an aperture appears in the video pane. Here is an example:



3. **Drag a side or corner of the box to change its size, shape and orientation to match that of the aperture image.**

   Here is an example:



Displaying a ruler

You can use the ruler tool to display a ruler for measuring items in the navigation pane or video pane. For example, if you want to measure the length of an item, you can draw a ruler alongside the item and the same length as the item. The length of the ruler displayed in the description bar is then the length of the item.

Follow these steps:

1. **Select the ruler tool.**

2. **Point to the location in the video pane where you want the ruler to start.**

3. **Press and hold down the mouse button.**

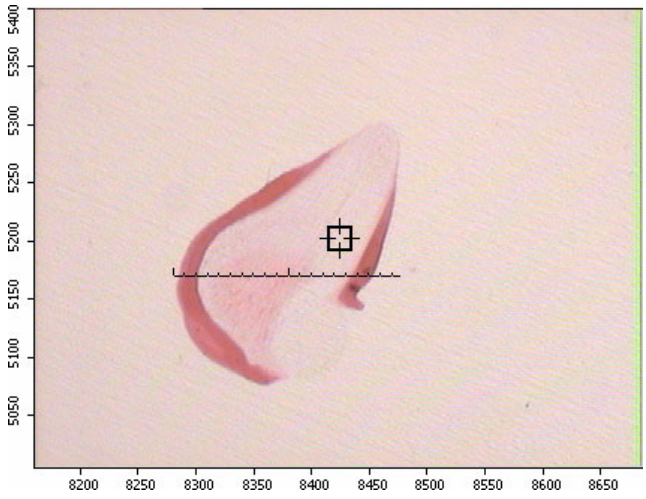
4. **Move the pointer to the location where you want the ruler to end.**

   The ruler changes in length and direction as you move the mouse.

5. **Release the mouse button.**

   If there was a ruler displayed in the pane, it is replaced by the new ruler.

Here is an example of a ruler drawn in the video pane:



The length of the new ruler appears in the description bar:

You can move or resize the ruler with the arrow tool as explained in "Moving the ruler" or "Resizing the ruler."

Adding text annotation

Follow the appropriate procedure below to add text annotation to the video pane or navigation pane.

Adding text annotation that is not connected with a line

Follow these steps to use the text tool to add text annotation that is not connected to the displayed item with a line:

1. **Select the text tool.**

2. **Turn off Connect Text Annotation With Lines on the Mapping tab of the Options dialog box.**

   See "Connecting text annotation with a line" for details.

3. **Click the location in the navigation pane or video pane where you want the text to begin.**

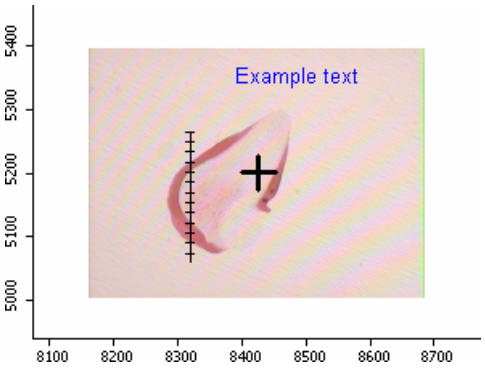
   A box appears:

4. **Type the desired text.**

   Pressing Enter on the keyboard begins a new line of text.

5. **Click outside the box.**

   The text annotation appears in the pane. Here is an example:



Adding text annotation that is connected with a line

Follow these steps to use the text tool to add text annotation that is connected to the displayed item with a line:

1. **Select the text tool.**

2. **Select Connect Text Annotation With Lines on the Mapping tab of the Options dialog box.**

   See “Connecting text annotation with a line” for details.

3. **Move the pointer over the location in the video pane where you want the line to begin.**

4. **Press and hold down the mouse button, move the pointer to the location where you want the line to end, and then release the mouse button.**

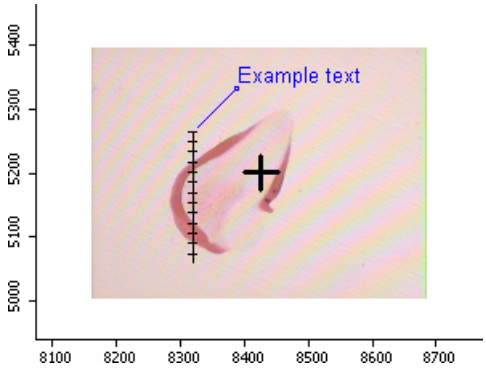
   A box appears:

5. **Type the desired text.**

   Pressing Enter on the keyboard begins a new line of text.

6. **Click outside the box.**

   The text annotation and connecting line appear in the pane. Here is an example:



Adding a marker

Use the marker tool to add markers to the navigation pane or video pane to identify locations of interest. This will help you find these locations later. Each marker appears as a consecutively numbered letter "M." Here is an example:

Follow these steps to add a marker:

1. **Select the marker tool.**

2. **Click the desired location in the navigation pane or video pane.**

   A new marker appears.

   You can drag the marker to a different location if desired. The marker moves in both panes when you drag it.

Moving maps and other items in the Atlμs window

The Atlμs window tool palette gives you great flexibility in moving items you have drawn in the window. The next sections explain how to move each type of item.

Moving a line map

Follow the steps below to move a line map without changing the length or slope of the map. See "Drawing a line map" for information about drawing line maps.

1. **Select the line map tool or arrow tool.**

2. **Move the pointer over the midpoint of the map so that the directional arrows shown below appear.**

3. **Drag the map to the desired location.**

   The next time you use Experiment Setup in the Collect menu, the information for the moved map will appear on the Mapping tab. See "Setting the mapping parameters" for details.

Moving an area map or box drawn to specify a Mosaic

Follow the steps below to move an area map without changing the size or shape of the map. You can also move a box drawn to specify a sample area for capturing a Mosaic. See "Drawing an area map (or Mosaic)" for information about drawing area maps.

1. **Select the area map tool or arrow tool.**

2. **Move the pointer over the center of the map (or box) so that the hand shown below appears.**

3. **Drag the map (or box) to the desired location.**

   The next time you use Experiment Setup in the Collect menu, the information for the moved map will appear on the Mapping tab. See "Setting the mapping parameters" for details.

Moving a discrete sample point or background point

Follow the steps below to move a discrete sample point or background point (if available). See "Specifying discrete sample points" or "Specifying a background point" for information about specifying points.

1. **Select the sample point tool, background point tool, arrow tool or marker tool.**

2. **Move the pointer over the point you want to move so that directional arrows shown below appear.**

3. **Drag the point to the desired location.**

   As you move the point, its new X and Y stage coordinates appear in the description bar.

If the point is a background point, its new location will appear on the Mapping tab the next time you use Experiment Setup in the Collect menu. See "Setting the mapping parameters" for details.

Moving the ruler

Follow these steps to move a ruler displayed within the video pane (see "Displaying a ruler"):

1. **Select the ruler tool or arrow tool.**

2. **Move the pointer over the center of the ruler, between the endpoints, so that the directional arrows shown below appear.**

3. **Drag the ruler to the desired location.**

Moving text annotation

Follow these steps to move text annotation created with the text tool (see "Adding text annotation"):

1. **Select the text tool or arrow tool.**

2. **If the text is not connected with a line, move the pointer over the beginning of the text so that the directional arrows shown below appear. If the text is connected with a line, move the pointer over the small box at the end of the line so that the arrows appear.**

3. **Drag the text to the desired location.**

   As you move the text, any line that was drawn with the text is adjusted for the new text location.

4. **Release the mouse button.**

   A box appears allowing you to edit the text if desired:

5. **To keep the current text, click outside the box. To edit the text, type the desired changes and then click outside the box.**

   While editing, you can press Enter on the keyboard to begin a new line of text. If you want to delete the text annotation completely, delete the text in the text box and then click outside the box.

Moving a marker

Follow these steps to move a marker you have added with the marker tool (see "Adding a marker"):

1. **Select the marker tool, arrow tool, sample point tool or background point tool (if available).**

2. **Move the pointer over the marker you want to move so that the directional arrows shown below appear.**

3. **Drag the marker to the desired location.**

Resizing maps and other items in the Atlμs window

After you have drawn an item in the Atlμs window, you can use different palette tools to resize the item. The next sections explain how.

Resizing a line map

Follow these steps to change the length or slope of a line map you have drawn with the line map tool (see "Drawing a line map"):

1. **Select the line map tool or arrow tool.**

2. **Move the pointer over the map endpoint you want to move so that directional arrows shown below appear.**

3. **Drag the endpoint to change the length and slope of the line as desired.**

   The next time you use Experiment Setup in the Collect menu, the information for the changed map will appear on the Mapping tab. See "Setting the mapping parameters" for details.

Note When you release the mouse button, the changed map may vary from the line you specified by dragging the endpoint. This is because the length of the map must be adjusted for the step size specified on the Mapping tab of the Experiment Setup dialog box (or to the aperture size default). See "Setting the data collection parameters for FT-IR and FT-Raman experiments" or "Setting the data collection parameters for visible Raman experiments" for more information.

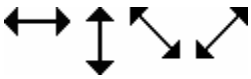
For example, if you used the mouse to specify a line map with a length of 100 micrometers and the step size is set to 22 micrometers, the length is automatically adjusted to 110 micrometers so that the step size is divided evenly into the map length. Map lengths always expand to compensate for step intervals; they are never less than the length you specified with the mouse. ▲

Resizing an area map or box drawn to specify a Mosaic

Follow the steps below to resize an area map. You can also resize a box drawn to specify a sample area for capturing a Mosaic (see "Capturing a Mosaic of video images for a sample area").

1. **Select the area map tool or arrow tool.**

2. **Move the pointer over the side or corner of the map (or box) you want to move so that one of the directional arrow pointers shown below appears.**



3. **Drag the side or corner until the map (or box) is the desired size and shape.**

   The next time you use Experiment Setup in the Collect menu, the information for the resized area map will appear on the Mapping tab. See "Setting the mapping parameters" for details.

Note When you release the mouse button, the resized map may vary from the area you specified by dragging. This is because the size of the map must be adjusted for the step size specified on the Mapping tab of the Experiment Setup dialog box (or to the aperture size default). See "Setting the data collection parameters for FT-IR and FT-Raman experiments" or "Setting the data collection parameters for visible Raman experiments" for more information.

For example, if you used the mouse to specify a new map area of 100 by 100 micrometers and the step size is set to 23 micrometers in both the X and Y dimensions, the map area is automatically adjusted to 115 by 115 micrometers so that the step size is divided evenly into the map area. Map areas always expand to compensate for step intervals; they are never less than the area you specified with the mouse. ▲

Resizing a drawn aperture

Follow the steps below to resize an aperture you have drawn within the video pane. The drawn aperture remains symmetrical about the center point. See "Drawing an aperture" for more information.

This section does not apply to Continuμm microscopes with the automated Reflex aperture. See "Setting the automated Reflex aperture" for information about adjusting that aperture.

1. **Select the aperture tool or arrow tool.**

2. **Move the pointer over a side or corner of the drawn aperture so that one of the pairs of directional arrows shown below appears.**

3. **Drag the side or corner until the drawn aperture is the desired size and shape.**

Note Adjust the aperture installed in the microscope to match the size, shape and orientation of the drawn aperture before collecting data. ▲

Resizing the ruler

Follow the steps below to resize a ruler you have drawn with the ruler tool. See "Displaying a ruler" for information about displaying a ruler.

1. **Select the ruler tool or arrow tool.**

2. **Move the pointer over the ruler endpoint you want to move so that directional arrows appear to the right of the pointer.**

3. **Drag the endpoint to change the length and slope of the ruler as desired.**

   If you are using the ruler tool, the new length of the ruler in micrometers appears in the description bar.

Deleting maps and other items in the Atlμs window

The Atlμs window tool palette gives you great flexibility in deleting items you have drawn in the window. The next sections explain how to delete each type of item. For information about deleting an entire map sequence, see "Clearing a map sequence."

Deleting a line map

Follow these steps to delete a line map you have drawn with the line map tool (see "Drawing a line map"):

1. **Select the line map tool or arrow tool.**
2. ***Right-click* the line map in the navigation pane or video pane.**
3. **Choose Delete Object or Delete Line Map from the pop-up menu.**

Deleting an area map

Follow these steps to delete an area map you have drawn with the area map tool (see "Drawing an area map (or Mosaic)"):

1. **Select the area map tool or arrow tool.**
2. ***Right-click* the area map in the navigation pane or video pane.**
3. **Choose Delete Object or Delete Area Map from the pop-up menu.**

Deleting a sample point

Follow these steps to delete a sample point you have specified with the sample point tool (see "Specifying discrete sample points"):

1. **Select the sample point tool or arrow tool.**
2. ***Right-click* the sample point in the navigation pane or video pane.**
3. **Choose Delete Object or Delete Sample Point from the pop-up menu.**

Deleting a background point

Follow these steps to delete a background point you have specified with the background point tool, if available (see "Specifying a background point"):

1. **Select the background point tool or arrow tool.**

2. ***Right-click*** **the background point in the navigation pane or video pane.**

3. **Choose Delete Object or Delete Background Point from the pop-up menu.**

Deleting a drawn aperture

Follow these steps to delete an aperture you have drawn with the aperture tool, if available (see "Drawing an aperture"):

1. **Select the aperture tool or arrow tool.**

2. ***Right-click*** **the drawn aperture in the video pane.**

3. **Choose Delete Aperture or Delete Object from the pop-up menu.**

Deleting a ruler

Follow these steps to delete a ruler you have drawn with the ruler tool (see "Displaying a ruler"):

1. **Select the ruler tool or arrow tool.**

2. ***Right-click*** **the ruler in the navigation pane or video pane.**

3. **Choose Delete Object or Delete Ruler from the pop-up menu.**

Deleting text annotation

Follow these steps to delete text annotation you added with the text tool (see "Adding text annotation"):

1. **Select the text tool or arrow tool.**

2. **Click the text annotation you want to delete.**

   The text becomes highlighted in a box. Here is an example:

3. **Press the Delete key on the keyboard.**

   The text is deleted from the box.

4. **Click outside the box.**

Deleting a marker


Follow these steps to delete a marker you have added with the marker tool (see "Adding a marker"):

1. **Select the marker tool or arrow tool.**

2. ***Right-click* the marker in the navigation pane or video pane.**

3. **Choose Delete Marker or Delete Object from the pop-up menu.**

Deleting all the displayed markers

Follow these steps to delete all the markers you have added with the marker tool (see "Adding a marker"):

1. **Select the marker tool.**

2. ***Right-click* anywhere in the navigation pane or video pane.**

3. **Choose Delete All Markers from the pop-up menu.**

Editing text annotation


Follow the steps below to edit text annotation created with the text tool or arrow tool (see "Adding text annotation").

1. **Select the text tool or arrow tool.**

2. **Click the text.**

   A box appears allowing you to edit the text:

3. **Type the desired changes.**

   While editing, you can press Enter on the keyboard to begin a new line of text. You can change the size of the box by dragging its sides or corners. If you want to delete the text annotation completely, delete all the text in the text box.

4. **Click outside the box.**

Rotating a drawn aperture

Follow the steps below to rotate an aperture you have drawn in the video pane (see “Drawing an aperture”).

This section does not apply to Continuμm microscopes with the automated Reflex aperture. See “Setting the automated Reflex aperture” for information about adjusting that aperture.

1. **Select the aperture tool or arrow tool.**

2. **Move the pointer over a corner of the drawn aperture so that one of the pairs of directional arrows shown below appears.**

3. **Drag the corner clockwise or counterclockwise until the drawn aperture is displayed at the desired angle.**

   You can drag in either direction up to a maximum of 45 degrees of rotation. With this range of rotation plus the ability you have to resize a drawn aperture with the aperture tool or arrow tool (see “Resizing a drawn aperture”), any combination of orientation and rectangular shape is possible.

Here is an example showing a drawn aperture that has been rotated:

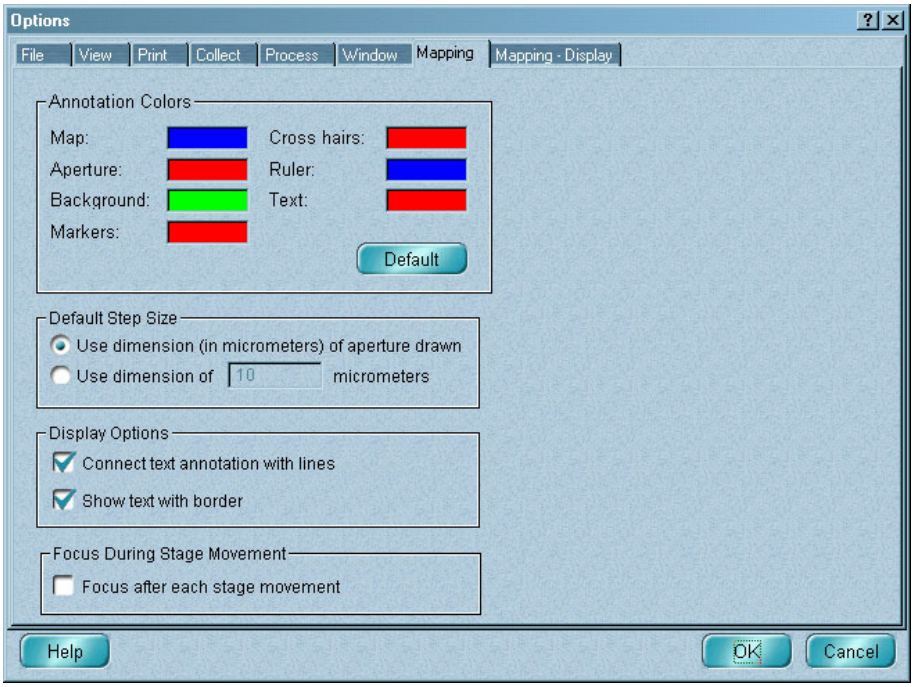
Note Adjust the aperture installed in the microscope to match the size, shape and orientation of the drawn aperture before collecting data. ▲

Setting the Mapping options

Use Options in the Edit menu to set several options that affect map data collection and the initial display of collected data in new map windows:

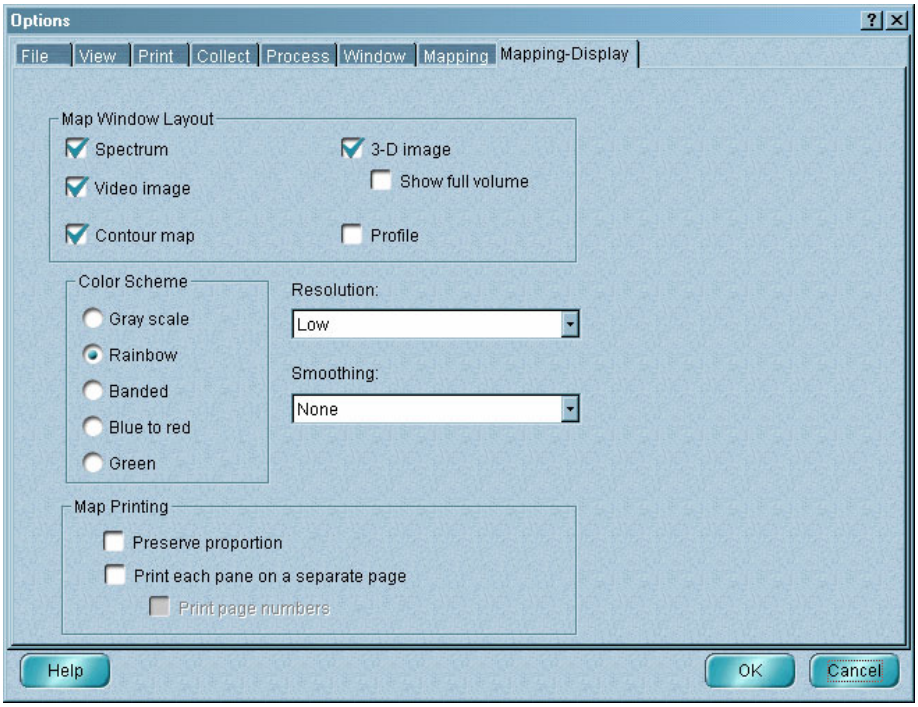
- Colors used to display annotation in the Atlμs window.
- A default step size for new map sequences.
- Whether to connect text annotation in the Atlμs window with a line.
- Whether to show a border around text annotation in the Atlμs window.
- Whether to focus the microscope automatically after each stage movement.
- The items to display in the map window.
- The color scheme to use for your contour map (or discrete point location map).
- The resolution for the contour map and 3-D image.
- The type of smoothing to use for the contour map.
- How to print map windows.

The options used to specify these items are on the Mapping tab...



...and the Mapping - Display tab in the Options dialog box:

The display options affect only new map windows created after future data collections. To change the way a map is displayed in an existing map window, use Display Setup in the View menu.



Follow the steps below to set the options. The individual options on the Mapping tab and the Map Printing options on the Mapping - Display tab are explained in the next sections. The rest of the options on the Mapping - Display tab work the same as options in the Display Setup dialog box. Resolution applies to the 3-D image and the contour map. Smoothing applies to the contour map; it also selects the Smoothing check box on the 3-D View tab of the Display Setup dialog box.

You can change the settings after data collection by using Display Setup in the View menu. See "Setting the display parameters" in the "Displaying Map Data" chapter for complete information about these options. In OMNIC Help Topics find "options" in the Index and go to "Customizing OMNIC by setting options" for information about the options on the other tabs.

1. **Choose Options from the Edit menu.**

   The Options dialog box appears.

2. **Select the Mapping tab.**

3. **Specify colors for the annotation types shown in the Annotation Colors box.**

   To change a color for an annotation type, click the color to the right of the type. The Color dialog box (a Windows feature) appears allowing you to select a color. If you need help using the features in this dialog box, click the "?" button and then click the feature of interest. When you are finished selecting a color, choose OK. The selected color appears to the right of the annotation type.

   To select the default colors for all the annotation types, click the Default button.

4. **Select the desired default step size option in the Default Step Size box.**

   - If you select Use Dimension (In Micrometers) Of Aperture Drawn, the default map step size will match the length of the shorter side of the current drawn aperture (if present).

   - If you select Use Dimension Of __ Micrometers, type the desired default map step size in the text box.

5. **If you want text annotation you create with the text tool to be connected to the annotated item with a line, select Connect Text Annotation With Lines in the Display Options box.**

6. **If you want text annotation you create with the text tool to have a border, select Show Text With Border in the Display Options box.**

7. **If you want the microscope focused automatically whenever you move the stage along the X-axis or Y-axis, select Focus After Each Stage Movement in the Focus During Stage Movement box.**

8. **Select the Mapping - Display tab and set the options as desired.**

   The Resolution parameter affects the contour map and the 3-D image. The Smoothing parameter affects the contour map. See “Setting the display parameters” in the “Displaying Map Data” chapter if you need help. This step is optional; you will be able to use Display Setup in the View menu to set the map display parameters after data collection.

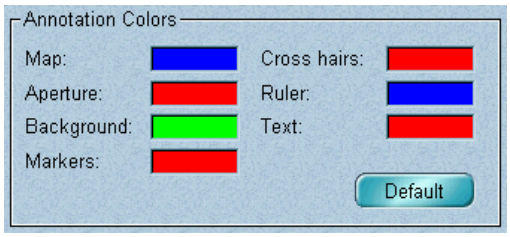
9. **Choose OK.**

   Any annotation that is displayed or that you create is displayed in the selected colors.

Specifying annotation colors

The features in the Annotation Colors box let you specify colors for displaying different types of annotation in the Atlμs window. Changing the color of annotation can make it easier to see against a similarly colored sample.

Initially the currently selected colors appear to the right of the listed annotation types. Here is an example:



The following table describes the available annotation types:

Annotation Type	Description
Map	Line maps, area maps and discrete sample points (including those in an ordered array) in the navigation and video panes.
Aperture	The box representing the automated Reflex aperture and a drawn aperture in the video pane. This feature does not apply to Nicolet Almega systems.
Background	Background points in the navigation and video panes. This feature does not apply to Nicolet Almega systems.
Markers	Markers in the navigation and video panes.
Cross Hairs	Cross hairs in the navigation and video panes.
Ruler	A ruler drawn in the navigation and video panes.
Text	Text annotation in the navigation and video panes.

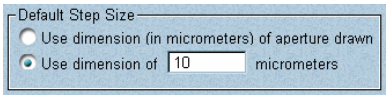
See the procedure in the preceding section for instructions for changing the colors of these annotation types.

You can click the Default button to return all the selected colors to the

default colors.

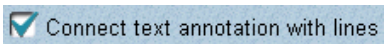
Your annotation color settings take effect when you choose OK to close the Options dialog box and are retained when you exit and restart OMNIC Atlμs.

Specifying a default step size



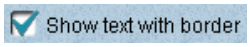
The options in the Default Step Size box let you specify the default step size (distance between adjacent sample points) for maps you define using the Mapping tab of the Experiment Setup dialog box or the palette tools. Select Use Dimension (In Micrometers) Of Aperture Drawn to specify a default step size that matches the length of the shorter side of the current drawn aperture (if you have created one). Select Use Dimension Of __ Micrometers if you want to enter a value in micrometers in the text box. Use this option if you have a Nicolet Almega system.

Connecting text annotation with a line



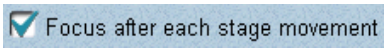
If you want text annotation you create in the navigation pane or video pane with the text tool to be connected to the annotated item with a line, select Connect Text Annotation With Lines in the Display Options box.

Displaying a border around text annotation



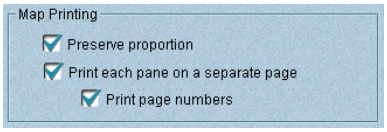
If you want a border displayed around text annotation, select Show Text With Border. Here is an example:

Focusing after each stage movement



If you want the microscope focused automatically whenever you move the stage along the X-axis or Y-axis, select Focus After Each Stage Movement in the Focus During Stage Movement box. You will be able to use autofocus when capturing a Mosaic with Capture Mosaic in the Atlμs menu.

Specifying how to print map windows



Use the options in the Map Printing box to specify how to print map windows:

Select Preserve Proportion if you want panes printed with the same proportion of height and width as is displayed in the window. If this option is not selected, the panes' proportions may be adjusted to fit the paper better.

Use Print Each Pane On A Separate Page to specify whether to print panes on separate pages or on the same page. If you select Print Each Pane On A Separate Page, use Print Page Numbers to specify whether to print page numbers on the pages.

Clearing a map sequence

Choose Clear Map Sequence from the Edit menu to remove the current map sequence and any drawn aperture or text annotation from the Atlμs window. All map sequence settings are also cleared from the Mapping tab of the Experiment Setup dialog box (see "Setting the data collection parameters for FT-IR and FT-Raman experiments" or "Setting the data collection parameters for visible Raman experiments" for more information).

Note If you have a Continuμm microscope with the automated Reflex aperture system, the box representing the Reflex aperture is not cleared. ▲

Note You can also use the arrow tool to clear a map sequence. Simply *right-click* anywhere in the navigation pane or video pane, and then choose Clear Sequence from the pop-menu. ▲

Tips Clearing a map sequence

- If you have not yet defined a new map sequence, you can undo the clear operation with Restore Map Sequence in the Edit menu. See "Restoring a cleared map sequence" for details.
- If you have collected a background spectrum using a material other than your sample, clear the background point and then move the sample into position and define the map. As long as you do not define a new background point for the map, the last background collected will be used to ratio the map spectra.

Restoring a cleared map sequence

If you have used Clear Map Sequence in the Edit menu to remove a map sequence from the Atlμs window and have not yet defined a new sequence, you can choose Restore Map Sequence from the menu to restore the sequence and its annotation. The settings on the Mapping tab of the Experiment Setup dialog box are also restored when you use Restore Map Sequence. See "Clearing a map sequence" for information about using Clear Map Sequence.

Saving a map sequence

Map sequence settings are saved in experiment files. To save the current map sequence and the other current experiment parameter settings, use the Save As button in the Experiment Setup dialog box (available through Experiment Setup in the Collect menu). Make sure the Map check box is selected in the Save Experiment As dialog box. If you are using OMNIC, choose OMNIC Help Topics from the Help menu, find "Experiment Setup command" in the Index and go to the "Using Experiment Setup" topic for more information. If you are using OMNIC For Raman, choose Raman Help Topics from the Raman menu, find "Experiment Setup command" in the Index and go to the "Setting the experiment parameters" topic.

Setting the data collection parameters for FT-IR and FT-Raman experiments

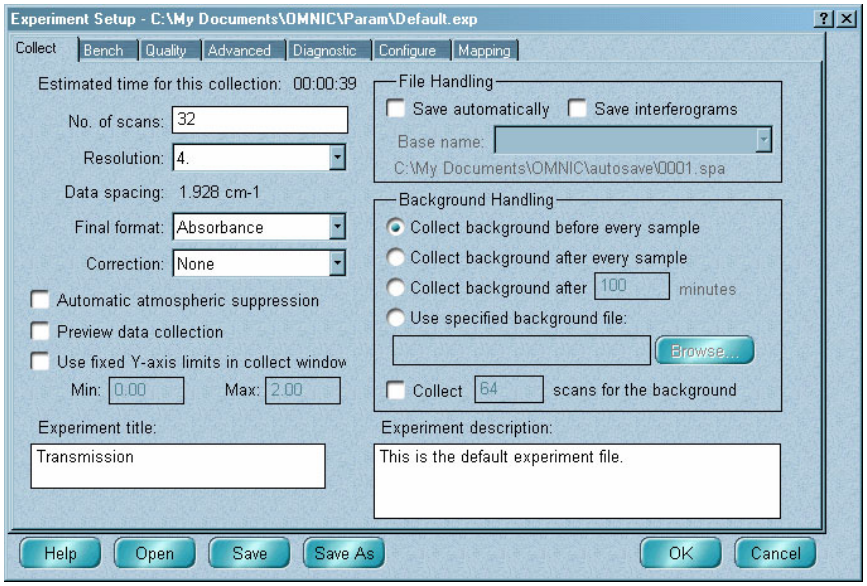
Use Experiment Setup in the Collect menu to set parameters that determine how a map is collected. This section covers only those parameters with special importance to map data collection. Complete information about the rest is available on-line. If you are using OMNIC, choose OMNIC Help Topics from the Help menu, find "Experiment Setup command" in the Index and go to the "Using Experiment Setup" topic. If you are using OMNIC For Raman, choose Raman Help Topics from the Raman menu, find "Experiment Setup command" in the Index and go to the "Setting the experiment parameters" topic. See "Setting the data collection parameters for visible Raman experiments" if you have a Nicolet Almega system.

Your settings determine the current map sequence. To save your settings in an experiment file that you can open later, use the Save As button in the Experiment Setup dialog box. See "Saving a map sequence" for more information.

Follow the general steps below to set the data collection parameters. The next sections explain the individual parameters in detail.

1. **Choose Experiment Setup from the Collect menu.**

   The Experiment Setup dialog box appears:



This dialog box has a slightly different appearance if you are collecting Raman data.

2. **Set the parameters as desired.**

   To display a set of parameters, click the appropriate tab.

3. **Choose OK.**

Tips

Setting the data collection parameters

When you set up map data collection, keep in mind that using a lower resolution (setting Resolution on the Collect tab to a higher number) increases the signal-to-noise ratio (SNR) of the data and may reduce the collection time. This can be an advantage over increasing the number of scans to improve the SNR.

When using the linear array detector, you should normally set the resolution to approximately 4 cm^{-1} (with Aperture set to 150). This will allow full illumination of the array detector and provide more uniform images. To avoid underfilling the linear array detector, do not set the resolution to a numerical value less than 1 cm^{-1} (with Aperture set to 34). To obtain images with the full detector array (28 elements), use a resolution in the range 16 to 4 cm^{-1}. To achieve resolutions better than 4 cm^{-1}, it is necessary to use an aperture size that may underfill the linear array detector. At resolutions greater than 4 cm^{-1} it is therefore necessary to limit the number of elements in the array that are used to collect the image. You can adjust this by using the Linear Array Setup button, available through the Collect button on the Mapping tab of the Experiment Setup dialog box. See “Setting special mapping options” for details.

When using the linear array detector within the spectral range 0 to 7899 cm^{-1} with a sample spacing of 2, set Velocity no higher than 2.5 cm/second. Within the range 15798 to 7900 cm^{-1} and with a sample spacing of 1, set Velocity no higher than 1.2.

Since the Aperture parameters are saved with the map sequence, setting them is a good way to keep a record of the aperture used for the experiment even if you are not using the aperture size to specify the step size for the map. You will be able to refer to the settings later when you view the map data.

Saving interferograms with the map

If you want interferograms to be saved with the map, select Save Interferograms on the Collect tab. The interferograms will be saved in one file whose name matches the file name of the map, except _IFG is added before the extension. For example, the interferograms for a map whose file name is POLY.MAP would be saved in a file named POLY_IFG.MAP.

Saving interferograms is necessary if you want to be able to reprocess the map later. See "Reprocessing a map" in the "Processing and Analyzing Map Data" chapter for more information.

Background handling

The options in the Background Handling box on the Collect tab let you specify when to collect a background or select a stored background to be used for ratioing map sample spectra. You can also specify the number of background scans to collect.

Note If you are collecting Raman data, the Reference Handling features appear instead of the Background Handling features. For information about these features, skip this section, find "reference" in the Index of Raman Help Topics and go to the "Reference handling" topic. ▲

Select Collect Background Before Every Sample if you want to collect a background before collecting each map spectrum.

Select Collect Background After Every Sample if you want to collect a background after collecting each map spectrum.

The Collect Background After __ Minutes option prompts you to collect a background after the specified number of minutes. Type the desired number of minutes in the box to the left of Minutes. You can use the Collect options (available through Options in the Edit menu) to specify how you will be prompted. (You will be prompted to collect a background the very first time you collect a map.) This option is useful when you use the same material (such as a gold mirror) for all of your background collections and don't need to collect a new background for each map.

To use a stored background, select Use Specified Background File. Type the name of the background file you want to use in the box next to Browse, or use the Browse button to select a background. This background will be used when collected map sample spectra are ratioed. You will not be able to collect a new background while this option is selected.

Note To store a background on a disk manually, use Collect Background in the Collect menu and then save the background spectrum using Save in the File menu. ▲

If the selected background is not adequate for the map you are collecting (because of a difference in resolution or data spacing), you will be prompted to collect a new background.

Typically the same number of scans are collected for both background and sample spectra. To improve the signal-to-noise ratio, you can collect a larger number of background scans by selecting Collect __ Scans For The Background and typing the desired number in the text box. When this option is selected, the Number Of Scans parameter affects only sample data collection.

Setting the gain

Set Gain on the Bench tab to control the amplification of the detector signal. Autogain is often a good choice. In OMNIC Help Topics or Raman Help Topics find "gain" in the Index and go to "Setting the gain" if you need more information.

Specifying the sample location and collection mode

Set Sample Compartment on the Bench tab to an appropriate setting described in the following table (only the settings that are appropriate for your system will be available).

Setting	Description
Right µScope; %T	Transmission experiment performed with the microscope installed to the right of the spectrometer.
Right µScope; %R	Reflection experiment performed with the microscope installed to the right of the spectrometer.
Left µScope; %T	Transmission experiment performed with the microscope installed to the left of the spectrometer.

Setting	Description
Left µScope; %R	Reflection experiment performed with the microscope installed to the left of the spectrometer.
Raman	Raman experiment performed with an FT-Raman View Stage in a Nicolet Nexus FT-Raman module.
Main	Raman experiment performed with an FT-Raman View Stage in either a Raman 960 spectrometer or Magna-IR™ FT-Raman module.

In OMNIC Help Topics find "beam path" in the Index and go to "Specifying the sample location" if you need more information. In Raman Help Topics find "beam path" in the Index and go to "Specifying the beam path."

Specifying the frequency range

Specify the frequency range (X-axis limits) of the data you want to save by setting Max Range Limit and Min Range Limit on the Bench tab. In OMNIC Help Topics or Raman Help Topics find "spectral range" in the Index and go to "Specifying the spectral range" if you need more information.

Specifying the detector for the Continuµm XL

If you have a Continuµm XL microscope and are preparing to perform an imaging experiment using the linear array detector, set Detector on the Bench tab to XL Array. This automatically sets Scope Aperture on the Bench tab to Imaging (see the next section).

Note Do not use the linear array detector for ATR experiments. ▲

See "Setting special mapping options" for information about specifying the elements of the linear array to use for data collection.

See the Tips at the end of "Setting the data collection parameters for FT-IR and FT-Raman experiments" for information about setting the resolution for the linear array detector.

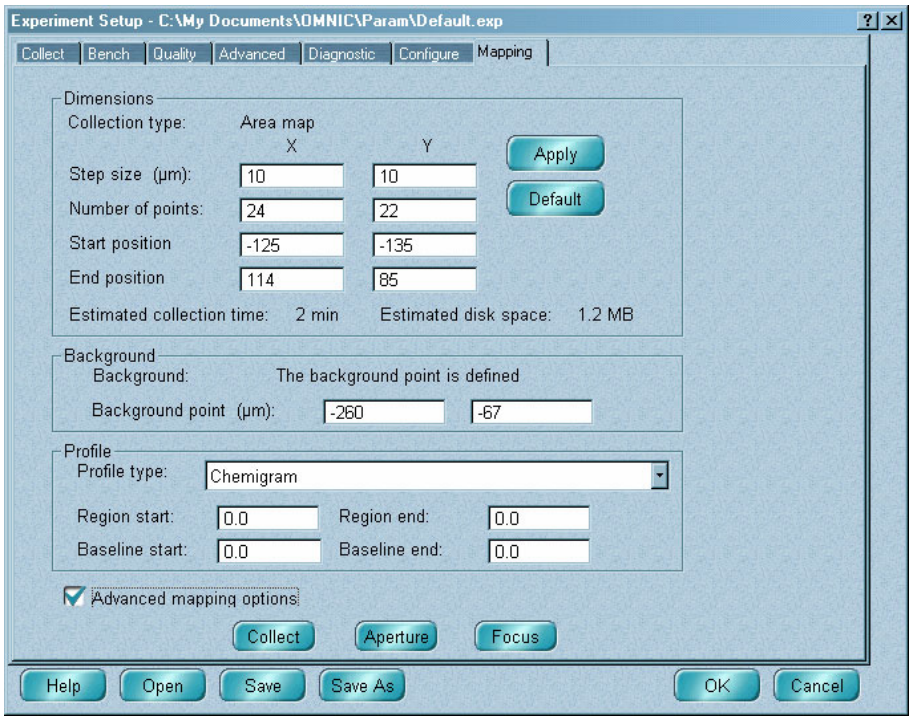
Setting the beam path for the Continuμm XL

If you have a Continuμm XL microscope, use Scope Aperture on the Bench tab to specify the beam path for your experiment. The following settings are available:

Setting	Description
Single	Uses the aperture before the sample (Target™ aperture) and the single-point detector.
Dual	Uses apertures before and after the sample (Reflex aperture) and the single-point detector.
Imaging	Uses the imaging beam path. The "Aperture mode" lights on the microscope front panel are off, because the apertures are not applicable for imaging. This setting is selected automatically when you set Detector on the Bench tab to XL Array (see the preceding section).

Setting the Mapping parameters

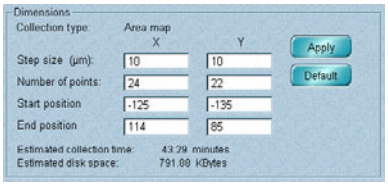
After you have specified a map using the Atlμs window palette tools (see "Specifying a map sequence" for details), you can use the parameters on the Mapping tab of the Experiment Setup dialog box to refine your specifications and specify a profile type. Here is an example showing the parameters set for collecting a map:



If you change a setting, the change is reflected in the map drawn in the Atlμs window when you choose Apply (if available) or choose OK to close the Experiment Setup dialog box.

The next sections explain how to set the parameters.

Setting the Dimensions parameters



The Dimensions parameters determine where and how map spectra will be collected.

The Collection Type readout shows the type of map you have specified with the Atlμs window palette tools (a line map, an area map or discrete points). The special parameters for each map type are discussed below.

- If you specified a *line map*, the Step Size (µm) text box in the X column (the Y column is not available) shows the distance in micrometers between consecutive sample points.

  The Number Of Points text box shows the number of sample points in the map.

- If you specified an *area map*, the Step Size (µm) text box in the X column shows the distance in micrometers between the columns of sample points in the map. The Step Size (µm) text box in the Y column shows the distance in micrometers between the rows of sample points.

  The Number Of Points text box in the X column shows the number of columns of points in the map. The Number Of Points text box in the Y column shows the number of rows of points.

- If you specified *discrete points*, the Number Of Points box shows the number of sample points.

  When specifying the step size, it is important to keep the aperture size in mind. You may wish to set the step size equal to the aperture size to ensure that spectra are obtained over the entire mapping region. You may also want to "over-step" your map to obtain a smoother profile. To do this, use a step size that is smaller than the aperture size.

  If Advanced Mapping Options (available only for line maps and area maps) is selected, the Start Position and End Position text boxes appear. They show the X and Y position values of the first and last sample points of the map, respectively. The X value of the end position should be greater than that of the start position (that is, to the right of the start position in the navigation or video pane).

  If you change a value in one of the text boxes in the Dimensions box and then choose Apply (if available) or OK, the values in the other text boxes are adjusted as needed to reflect the change you made and to allow even spacing of points.

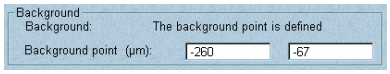
  Estimates of the total collection time and the amount of disk space that will be needed to store the spectra appear at the bottom of the Dimensions box when you choose Apply.

You should generally try to minimize the time needed to collect a map. Decreasing the number of scans, decreasing the spectral resolution (for example, changing from 4 wavenumbers to 8 wavenumbers) and increasing the step size can all reduce the total collection time. (The Resolution parameter is on the Collect tab.) Conversely, the number of scans and the aperture size should be large enough to give high signal-to-noise values, and the step size should not be so large as to sacrifice spatial resolution. Use the combination of settings that provides the best compromise for your experiment.

Click the Default button if you want to set the step sizes and number of points to zero and set the background point to undefined.

Note If you specify an ordered array of discrete points, you enter the step size and number of points just after drawing the array. See "Specifying an ordered array of discrete points" for details. ▲

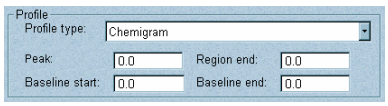
Setting the Background parameters



The Background parameters determine where the map background spectrum will be collected. If you have specified a background point with the background point tool, the X and Y position values of the point appear in the Background Point (µm) text boxes, in that order. You can specify new values by typing in the text boxes.

If you have selected Use Specified Background File on the Collect tab, the Background Point (µm) text boxes are not available. See "Background handling" for information about using a stored background.

Setting the Profile parameters



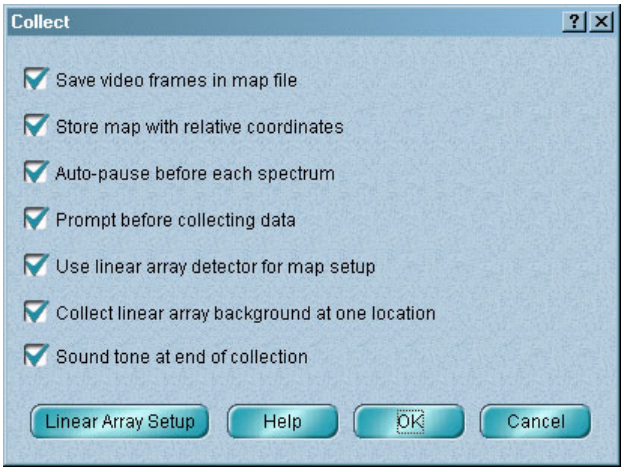
The Profile parameters (available only for area maps) let you specify a profile before data collection. The term "profile" is used to refer to any of the ways of representing map data described in the table in the "Creating a profile" section in the "Processing and Analyzing Map Data" chapter. See that section for details on the available profile types, including the information you need to enter for each. If you don't specify a profile type, the default profile will be used: Chemigram. For the profile types that use two peaks, "Peak 2" is the ratio denominator.

Note Specifying the profile type before data collection is entirely optional. After you collect the map, you will be able to use Profile Setup in the Atlμs menu to create profiles. ▲

Note The Functional Group and Correlation Map profile types are not available before data collection. ▲

Setting special mapping options

Use the Collect button on the Mapping tab to display and select the special mapping options shown below and to set up the linear array.



The following table shows what you can specify with each option. The Linear Array Setup button is explained later in this section.

Option	Description
Save Video Frames In Map File	Select this option if you want the video frames for maps saved in the map file. Since map files are much larger when they include stored video information, you should save the video frames only if you have adequate disk space. If you have specified discrete sample points or an ordered array of points, you can use the sample point tool to specify that the video image for an individual sample point not be captured and saved. See “Capturing and saving the video image for sample points” for details.

Option	Description
Store Map With Relative Coordinates	Select this option if you want relative coordinates used instead of actual stage positions as grid references for the spectral data when the contour map (or discrete point location map) is displayed. When relative coordinates are used, the first point collected (the start point) becomes 0,0. Relative coordinates are useful when you are running a similar sample repeatedly, but its position relative to the stage is changing. This option lets you directly compare these samples.
Auto-Pause Before Each Spectrum	Select this option if you want the system to pause after each sample spectrum is collected and again after the stage is moved to the next sample point. This is useful when you are collecting ATR data and need to release contact after a spectrum is collected and reestablish contact before the next spectrum is collected. Pausing is also useful when the sample is uneven, requiring you to refocus at some of the sample points.
Prompt Before Collecting Data	Select this option if you want the software to display a prompt immediately before collecting the first map spectrum. This option is useful if you want to save the video frames without an aperture in place but need to use an aperture during data collection. This option is also useful if you need to change the focus before starting sample collection when background collection is finished. In addition, if your microscope does not have automated mirrors controlled by the software and you want to save the video frames, you must select this option so that you can flip the mirrors manually before the first spectrum is collected. Follow these steps to use this option: 1. Set up the mapping experiment with the aperture in place. Select the Save Video Frames In Map File option. 2. Remove the aperture. 3. Initiate map data collection with Collect Map. 4. When the prompt appears, install the aperture (and manually flip the microscope mirrors if they are not automated) and then choose OK.

Option	Description
Use Linear Array Detector For Map Setup	Changes the map collection ranges to match the linear array configuration specified with the Linear Array Setup button (explained below). This option also displays in the navigation pane a background cursor that shows the size and shape of the linear array configuration, with the background area inside the box. Here is an example:  This lets you position the background point so that the area of the linear array does not overlap the area where you will collect sample data. This option is available only if your system can perform linear array collections.
Collect Linear Array Background At One Location	When the background is collected, the background point (shown in the center of the box) is moved under each detector element in the linear array instead of collecting the background at all of the detector element positions shown with the background cursor (displayed by Use Linear Array Detector For Map Setup). The additional stage movement increases the collection time. This option is available only if your system can perform linear array collections.
Sound Tone At End Of Collection	Emits a tone when map data collection is finished.

If your system can perform linear array collections, use the Linear Array Setup button to specify the elements to use for data collection.

You can also specify that oversampling be used to improve spatial resolution. Oversampling has several advantages over using hardware enhancements to achieve this improvement:

- There is no need for multiple optics or detectors.

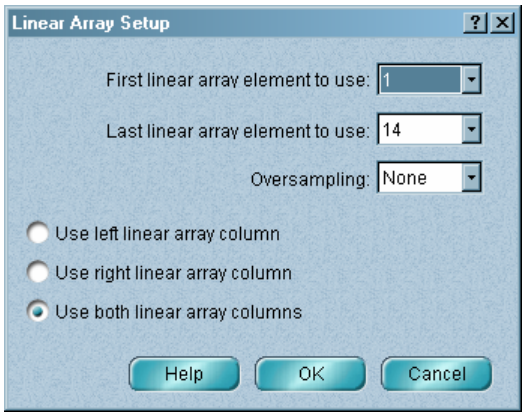
- Each detector element views a sample area that is independent of resolution. Therefore, unlike with hardware enhancements, the signal-to-noise ratio remains high.

- Since it is controlled through software rather than hardware, the degree of oversampling is adjustable.

Follow these steps to set up the linear array:

1. **Click the Linear Array Setup button.**

   The Linear Array Setup dialog box appears:



2. **Specify the range of linear array elements to use for data collection.**

   The array has two parallel columns of 14 elements each. The elements in each column are numbered 1 through 14. Data collection will be performed using the specified range of elements in the column or columns that you specify in the next step. Also, if you select Use Linear Array Detector For Map Setup in the Collect dialog box (explained earlier in this section), the size and shape of the rectangular background cursor is determined by the elements you have specified.

   Select the first element to use from the first drop-down list box and the last element to use from the second drop down list box. To use just one element per column, select the same number from both drop-down list boxes.

3. **Specify the amount of oversampling to use by setting Oversampling.**

   Normally (with Oversampling set to None) the system moves the sample the full width of an array element before collecting data at the next position for a map. This results in no overlap of measured sample areas. When you collect data with oversampling, the system uses partially overlapped sample areas. This overlap results in improved spatial resolution.

   For example, if you set Oversampling to 4X, the system will "subdivide" the element area into a grid of four equal parts and move the sample to center it on each of these parts before collecting data in that position. As a result, any point on the mapped sample area is sampled four times.

4. **Specify the column or columns to use by selecting the appropriate option button.**

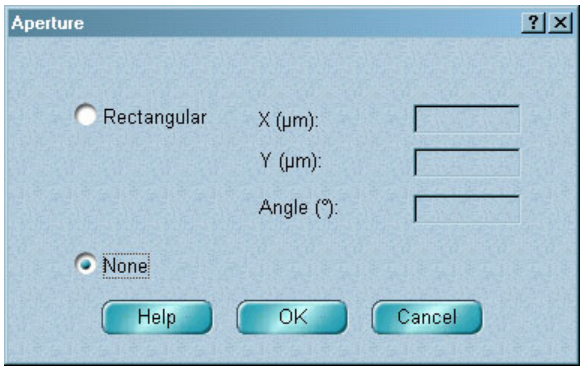
Note You may need to use only one column if your sample alignment does not uniformly illuminate both columns. This may more likely occur in reflection mode and result in vertical stripes in the image. ▲

5. **Choose OK.**

   When you are finished using the Collect dialog box, choose OK.

Specifying the automated Reflex aperture

Use the Aperture button on the Mapping tab to specify the size, shape and orientation of the automated Reflex aperture on a Continuμm microscope. When you click the button, the Aperture dialog box appears:



The rectangular aperture settings in this dialog box are linked to those in the dialog box displayed by Aperture Dimensions from the Atlμs menu. See "Setting the automated Reflex aperture numerically" for more information.

To specify the aperture, select Rectangular. The aperture parameters become available. The following table describes the parameters. If you are not using a Reflex aperture, select None if it is not already selected.

Parameter	Description
X (μm)	The X dimension of the aperture in micrometers, before any rotation.
Y (μm)	The Y dimension of the aperture in micrometers, before any rotation.
Angle (°)	The angle by which the aperture is rotated about the map center point within the plane of the sample. An angle of 0 positions the aperture with its X dimension parallel to the X-axis. You can rotate the aperture from 45 to -45 degrees (a negative angle rotates the aperture clockwise). With this range of rotation plus the ability to specify the size of the aperture, any combination of orientation and rectangular shape is possible.

When you are finished setting the aperture parameters, choose OK.

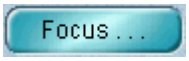
Important Use only the software to adjust the aperture; do *not* use the Reflex aperture control knobs on the microscope. If you do adjust the knobs, you can reset the aperture by using the Aperture button in the System Configuration dialog box. See "Initializing the automated Reflex aperture" in the "Configuring the System" chapter for details. Follow these precautions: If the microscope has a motorized stage or the autofocus option, remove the nosepiece and lower the condenser all the way before turning on the power. After the microscope has initialized, reinstall the nosepiece. ▲

Note The minimum size of the automated Reflex aperture is nominally 10 by 10 micrometers. If you attempt to set the aperture to this or a smaller size, the system will automatically adjust the aperture to the minimum size possible on your microscope (typically 8 by 8 micrometers). The minimum available size varies slightly from system to system. ▲

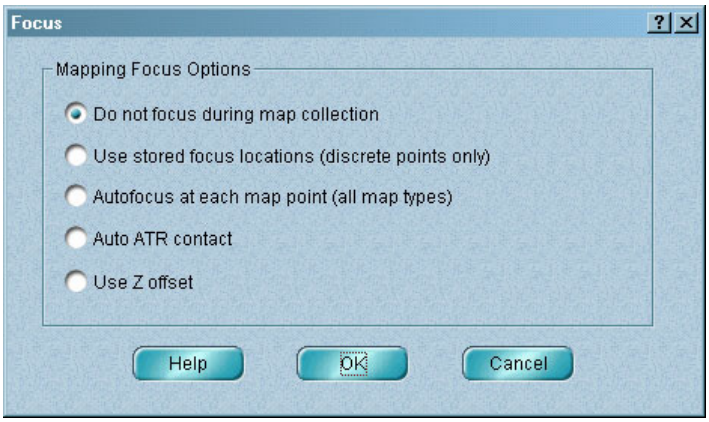
For more information about the Reflex aperture, see the documentation that came with your microscope.

Note You can also adjust the aperture graphically in the video pane as explained in "Adjusting the automated Reflex aperture graphically." You can use Set Aperture To Default in the Atlμs menu to set the aperture to its default size, shape and orientation as explained in "Setting the automated Reflex aperture to the default." ▲

Setting the focus parameters



Use the Focus button on the Mapping tab to display and set the focus options shown below. They control whether and how the microscope is focused automatically during data collection.



Note The Focus button is available only if your microscope has the required hardware. Only the options that are appropriate for your hardware configuration are available. ▲

The following table shows the effect of each option.

Selecting this option…	Has this effect…
Do Not Focus During Map Collection	The microscope is not focused during map collection.
Use Stored Focus Locations (Discrete Points Only)	The microscope is focused at the discrete point locations you specified (including those in an ordered array). Select this option only if you are collecting data at discrete points rather than a line map or area map. You can specify the focus location (Z position) for a discrete sample point. See "Setting the Z position for a discrete point to the current Z position" for more information. If you have a Centaurμs microscope with an XL stage with motorized Z-axis movement, use only the stage controller or focus buttons in the Atlμs window to adjust the focus when using this option. The stage coarse and fine focus knobs do not update the Z value.
Autofocus At Each Map Point (All Map Types)	The microscope is focused at each location where data is collected. You can use this option for any type of data collection.
Auto ATR Contact	The microscope automatically makes and releases contact with the sample at each sample point. Contact is not made automatically for the background collection. See "Using auto ATR contact" in the "Collecting Data" chapter for more information.

When you are finished setting the options, choose OK.

Setting the data collection parameters for visible Raman experiments

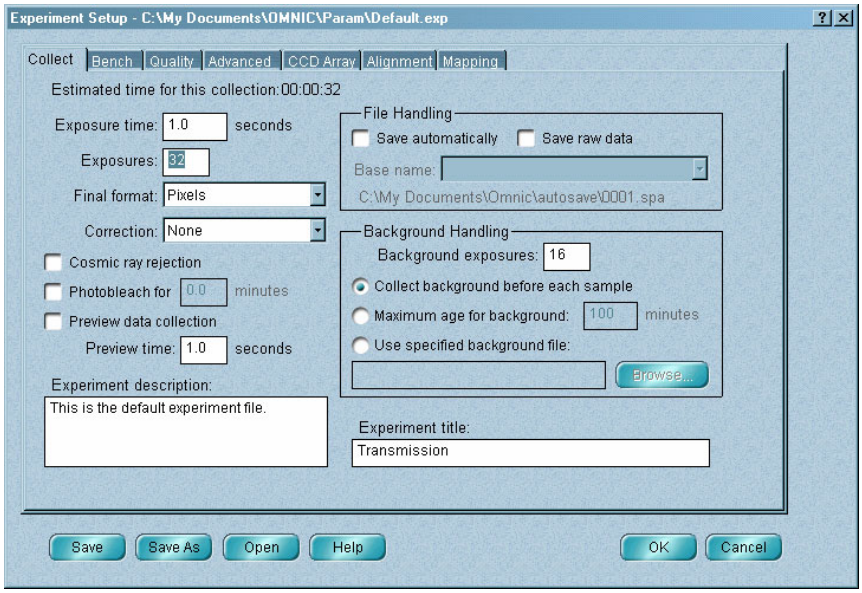
Use Experiment Setup in the Collect menu to set parameters that determine how a map is collected. This section covers only those parameters with special importance to map data collection. Complete information about the rest is available on-line. Choose OMNIC Help Topics from the Help menu, find "Experiment Setup command" in the Index and go to the "Using Experiment Setup" topic. See "Setting the data collection parameters for FT-IR and FT-Raman experiments" if you have an FT-IR or FT-Raman system.

Your settings determine the current map sequence. To save your settings in an experiment file that you can open later, use the Save As button in the Experiment Setup dialog box. See "Saving a map sequence" for more information.

Follow the general steps below to set the data collection parameters. The next sections explain the individual parameters in detail.

1. **Choose Experiment Setup from the Collect menu.**

   The Experiment Setup dialog box appears:



2. **Set the parameters as desired.**

   To display a set of parameters, click the appropriate tab.

3. **Choose OK.**

Tips Setting the data collection parameters

- When you set up map data collection, keep in mind that using a lower resolution increases the signal-to-noise ratio (SNR) of the data and may reduce the collection time. This can be an advantage over increasing the number of scans to improve the SNR.

Specifying the sample location

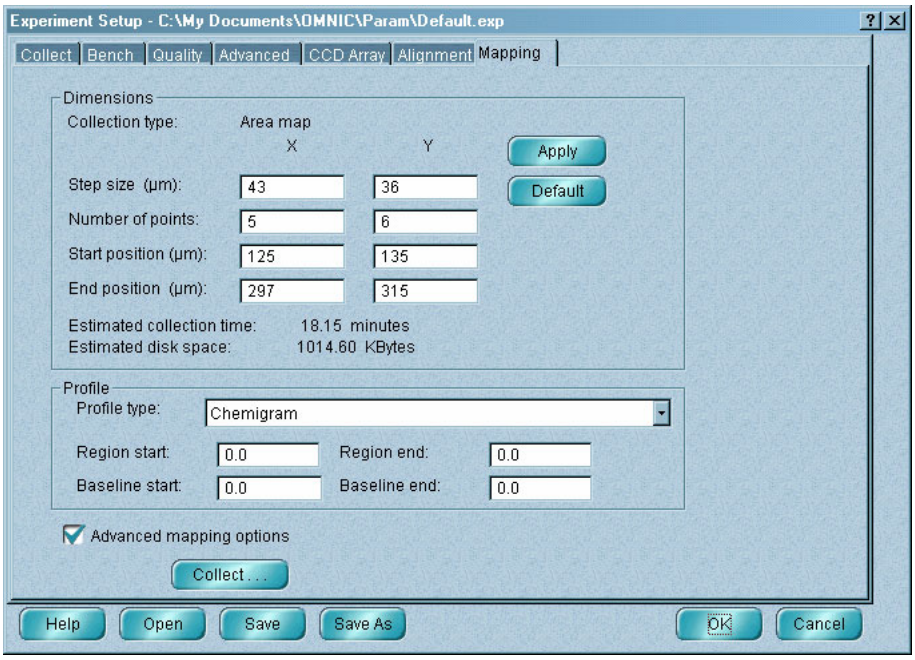
Specify the sample location by selecting Microscope in the Beam Path/Sample Position box on the Bench tab.

Specifying the spectral range

Specify the spectral range (X-axis limits) of the data to save by setting Spectral Range on the Bench tab. In OMNIC Help Topics find "spectral range" in the Index and go to "Specifying the spectral range" if you need more information.

Setting the Mapping parameters

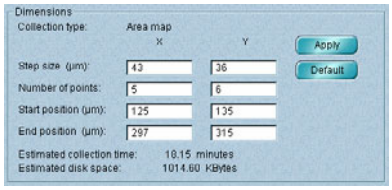
After you have specified a map using the Atlμs window palette tools (see "Specifying a map sequence" for details), you can use the parameters on the Mapping tab of the Experiment Setup dialog box to refine your specifications and specify a profile type. Here is an example showing the parameters set for collecting a map:



If you change a setting, the change is reflected in the map drawn in the Atlμs window when you choose Apply (if available) or choose OK to close the Experiment Setup dialog box.

The next sections explain how to set the parameters.

Setting the Dimensions parameters



The Dimensions parameters determine where and how map spectra will be collected.

The Collection Type readout shows the type of map that will be collected. The special parameters for each of these types are discussed below; the parameters for specifying a depth profile are discussed under "Specifying a depth profile."

- If you specified a *line map*, the Step Size (μm) text box in the X column (the Y column is not available) shows the distance in micrometers between consecutive sample points.

The Number Of Points text box shows the number of sample points in the map.

- If you specified an *area map*, the Step Size (µm) text box in the X column shows the distance in micrometers between the columns of sample points in the map. The Step Size (µm) text box in the Y column shows the distance in micrometers between the rows of sample points.

  The Number Of Points text box in the X column shows the number of columns of points in the map. The Number Of Points text box in the Y column shows the number of rows of points.

- If you specified *discrete points*, the Number Of Points box shows the number of sample points.

  If Advanced Mapping Options (available only for line maps, area maps and depth profiles) is selected, the Start Position and End Position text boxes appear. For a line map or area map they show the X and Y position values of the first and last sample points of the map, respectively. The X value of the end position should be greater than that of the start position (that is, to the right of the start position in the navigation or video pane).

  If you change a value in one of the text boxes in the Dimensions box and then choose Apply (if available) or OK, the values in the other text boxes are adjusted as needed to reflect the change you made and to allow even spacing of points.

  Estimates of the total collection time and the amount of disk space that will be needed to store the spectra appear at the bottom of the Dimensions box when you choose Apply.

  You should generally try to minimize the time needed to collect a map. Decreasing the number of exposures, decreasing the spectral resolution (for example, changing from 4 wavenumbers to 8 wavenumbers) and increasing the step size can all reduce the total collection time. (The Resolution parameter is on the Collect tab.) Conversely, the number of exposures should be large enough to give high signal-to-noise values, and the step size should not be so large as to sacrifice spatial resolution. Use the combination of settings that provides the best compromise for your experiment.

Click the Default button if you want to set the step sizes and number of points to zero and set the background point to undefined.

Note If you specify an ordered array of discrete points, you enter the step size and number of points just after drawing the array. See "Specifying an ordered array of discrete points" for details. ▲

Specifying a depth profile

There are two kinds of depth profile:

A line depth profile contains spectra collected at evenly spaced points arranged in a vertical column within the sample. This is similar to a line map that has been rotated to a vertical orientation.

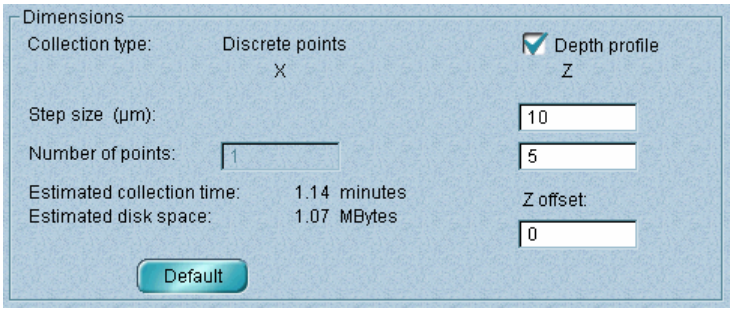
An area depth profile contains spectra collected at evenly spaced points in a series of evenly spaced vertical columns within the sample. This is similar to an area map that has been rotated to lie within a vertical plane.

Depending on the current stage position and whether you specify a Z offset, both of these profile types may include spectra collected above the sample or at its surface.

Specify the number and location of sample points for a depth profile as explained below.

Note The Depth Profile check box is not available if more than one discrete sample point has been specified in the Atlμs window. ▲

- To specify a *line depth profile*, use the sample point tool to click the desired location in the navigation pane or video pane *before* choosing Experiment Setup. When you display the Mapping tab and select Depth Profile, these parameters appear:

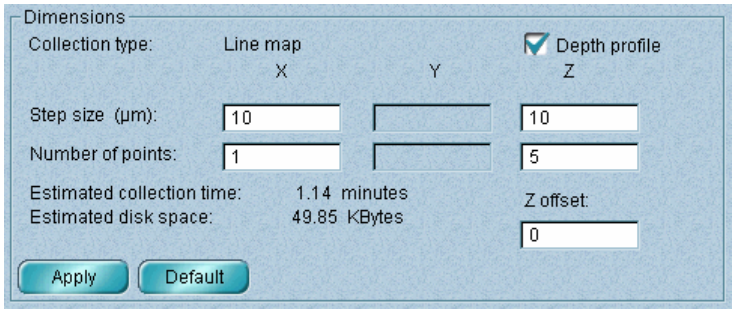


Type the desired step size in the Step Size (µm) in the Z column. This determines the distance between the sample points.

Type the desired number of sample points in the Number Of Points text box in the Z column.

If you have selected Use Z Offset in the Focus dialog box (see "Setting the focus parameters"), type the desired Z offset in the Z Offset text box. This determines the vertical distance from the current Z position that the first sample spectrum will be collected. This is useful when you want to collect some of the data above the sample surface. Enter a positive value to collect the first spectrum above the current position. Enter a negative value to collect the spectrum below the current position. Enter 0 to collect the spectrum at the current Z position. The current Z position is displayed in the description bar in the Atlµs window.

- To specify an *area depth profile*, use the line map tool to draw a line in the desired location in the navigation pane or video pane and then choose Experiment Setup. (If you prefer not to draw a line, you can just enter endpoint coordinates on the Mapping tab.) When you display the Mapping tab and select Depth Profile, these parameters appear:



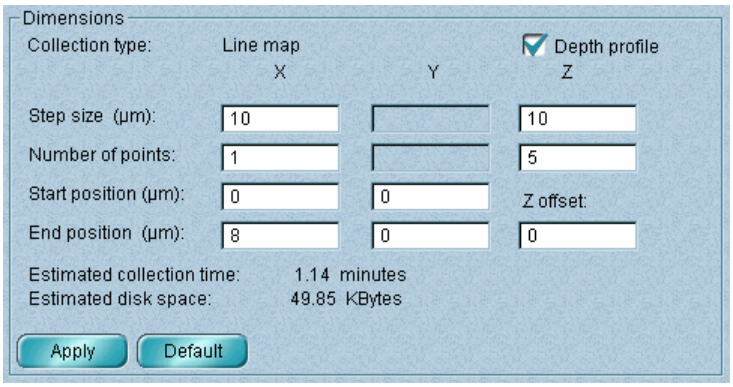
Type the desired horizontal step size in micrometers in the Step Size (µm) text box in the X column. This determines the distance between the vertical columns of points.

Type the desired vertical step size in micrometers in the Step Size (µm) text box in the Z column. This determines the distance between the horizontal rows of points.

Type the desired number of vertical columns of points in the Number Of Points text box in the X column.

Type the desired number of horizontal rows of points in the Number Of Points text box in the X column.

If you select Advanced Mapping Options, additional parameters appear:

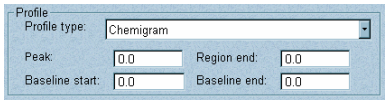


Type the desired X and Y values of the first point in the Start Position (µm) text boxes in the X and Y columns.

Type the desired X and Y values of the last point in the End Position (µm) text boxes in the X and Y columns.

Type the desired Z offset in the Z Offset text box. See the discussion of Z Offset above for more information.

Setting the Profile parameters



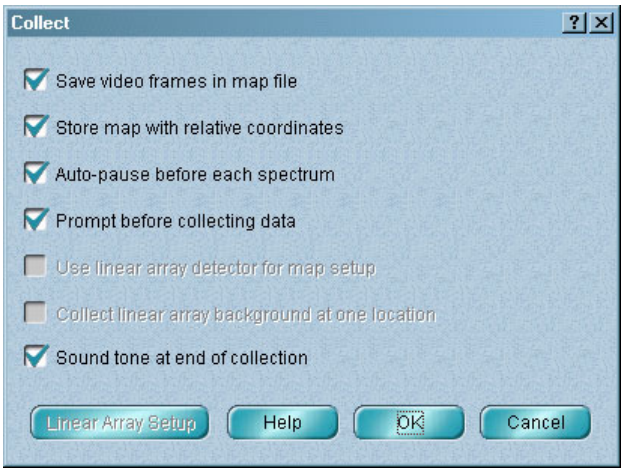
The Profile parameters (available only for area maps) let you specify a profile before data collection. The term "profile" is used to refer to any of the ways of representing map data described in the table in the "Creating a profile" section in the "Processing and Analyzing Map Data" chapter. See that section for details on the available profile types, including the information you need to enter for each. If you don't specify a profile type, the default profile will be used: Chemigram. For the profile types that use two peaks, "Peak 2" is the ratio denominator.

Note Specifying the profile type before data collection is entirely optional. After you collect the map, you will be able to use Profile Setup in the Atlµs menu to create profiles. ▲

Note The Functional Group and Correlation Map profile types are not available before data collection. ▲

Setting special mapping options

Use the Collect button on the Mapping tab to display and select the special mapping options shown below.



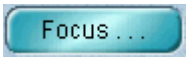
The following table shows what you can specify with each available option (the linear array options are not available for visible Raman experiments).

Option	Description
Save Video Frames In Map File	Select this option if you want the video frames for maps saved in the map file. Since map files are much larger when they include stored video information, you should save the video frames only if you have adequate disk space. If you have specified discrete sample points or an ordered array of points, you can use the sample point tool to specify that the video image for an individual sample point not be captured and saved. See “Capturing and saving the video image for sample points” for details.
Store Map With Relative Coordinates	Select this option if you want relative coordinates used instead of actual stage positions as grid references for the spectral data when the contour map (or discrete point location map) is displayed. When relative coordinates are used, the first point collected (the start point) becomes 0,0. Relative coordinates are useful when you are running a similar sample repeatedly, but its position relative to the stage is changing. This option lets you directly compare these samples.

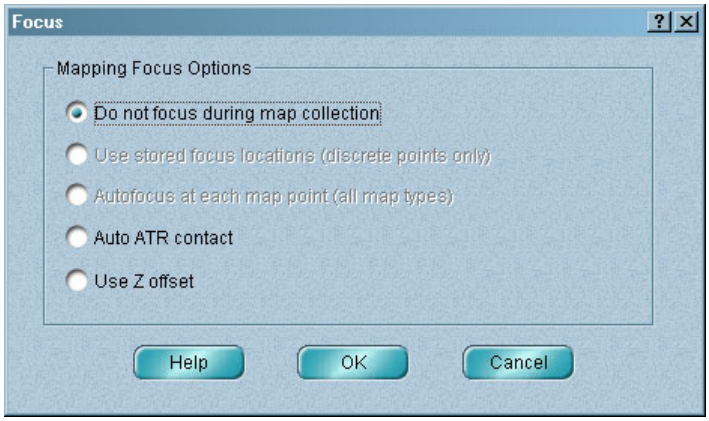
Option	Description
Auto-Pause Before Each Spectrum	Select this option if you want the system to pause after each sample spectrum is collected and again after the stage is moved to the next sample point. Pausing is useful when the sample is uneven, requiring you to refocus at some of the sample points.
Prompt Before Collecting Data	Select this option if you want the software to display a prompt immediately before collecting the first map spectrum.
Sound Tone At End Of Collection	Emits a tone when map data collection is finished.

When you are finished selecting options, choose OK.

Setting the focus parameters



Use the Focus button on the Mapping tab to display and set the focus options shown below. They control whether and how the microscope is focused automatically during data collection.



Note The Focus button is available only if your microscope has the required hardware. Only the options that are appropriate for your hardware configuration are available. ▲

The following table shows the effect of each available option.

Selecting this option…	Has this effect…
Do Not Focus During Map Collection	The microscope is not focused during map collection.
Use Stored Focus Locations (Discrete Points Only)	The microscope is focused at the discrete point locations you specified (including those in an ordered array). Select this option only if you are collecting data at discrete points rather than a line map or area map. You can specify the focus location (Z position) for a discrete sample point. See "Setting the Z position for a discrete point to the current Z position" for more information. If your microscope has motorized Z-axis movement, use only the stage controller or focus buttons in the Atlμs window to adjust the focus when using this option. The stage coarse and fine focus knobs do not update the Z value.
Autofocus At Each Map Point (All Map Types)	The microscope is focused at each location where data is collected. You can use this option for any type of data collection.
Use Z Offset	If you selected Save Video Frames In Map File in the Collect dialog box (see "Setting special mapping options") and want to use video and sample focus locations that are a fixed distance apart, select Use Z Offset. This is useful for samples whose optimum focus location for collecting data is some known distance below the sample surface. Specify this distance, or "offset," by typing a value in micrometers in the Z Offset text box on the Mapping tab. At each sample point the software will focus on the sample surface and capture a video image, move the focus location into the sample the specified distance, and then collect the data.

When you are finished setting the options, choose OK.

Working with video images and Mosaics

OMNIC Atlμs provides features for working with video images of sample surfaces and Mosaics made up of multiple video images. The next sections explain how to perform the following tasks with these images in the Atlμs window:

- Specify that the video image at a sample point be captured and saved with the spectrum for that point.
- Save a video image as a bitmap file.
- Capture and display a Mosaic of video images.
- Clear a Mosaic from the Atlμs window.
- Copy a Mosaic to the Windows Clipboard.
- Save a Mosaic as a bitmap file.

Capturing and saving the video image for sample points

If you are collecting data at discrete sample points, you can use the sample point tool to specify whether the video image at the specified sample points is captured and saved with the spectra for those points when you collect data. You will be able to view the saved images when you view the collected map in a map window. Follow these steps:

1. **Select the sample point tool.**

2. ***Right-click* a sample point in the navigation pane or video pane.**

3. **Choose Toggle Capture Video For Sample Point from the pop-up menu.**

   An asterisk (*) appears next to the point's number to indicate that a video image will be captured and saved for that point. Here is an example:

   You can remove the asterisk, and cancel the capture of the video image, by repeating steps 2 and 3.

Tips Saving the video image for sample points

- The video image is captured using the same pixel resolution as the displayed image.
- To specify whether to capture and save video images for all sample points for any type of map, select Save Video Frames In Map File, available through the Collect button on the Mapping tab of the Experiment Setup dialog box. See "Setting special mapping options" for details.

Saving the video image

Use Save Video Image in the File menu to save the video image displayed in the video pane of the Atlμs window or the active map window, at its current size, as a 24-bit, true-color, bitmap (.BMP) file. Any displayed annotation, cross hairs and axes are included when you save the image. You can open the file later using an application that opens bitmap files.

Follow these steps to save the video image:

1. **Adjust the display of the video image as desired.**
2. **Choose Save Video Image from the File menu.**

   The Save As dialog box appears.
3. **Type a file name in the File Name text box.**
4. **Locate and open the directory where you want the image saved.**
5. **Choose OK.**

Tips Saving the video image

- The video image is saved using the same pixel resolution as the displayed image.

Using Mosaics

You can capture a Mosaic of video images of a sample area and display it in the navigation pane. This is useful when you are defining a map that is larger than one video frame or want a video record of a large sample area. The Mosaic will also appear in the video pane of the map window when you later display the collected map. The next sections explain how to capture, clear, copy and save a Mosaic.

Capturing a Mosaic of video images for a sample area

Use Capture Mosaic in the Atlμs menu to capture a Mosaic of video images within a specified area of the sample and display it in the navigation pane as one image of the entire area.

When you capture a Mosaic, the software moves the stage to position each portion of the specified area under the objective so that a video frame can be captured and stored for later assembly. If you selected Focus After Each Stage Movement on the Mapping tab of the Options dialog box, the system automatically focuses each frame before it is captured.

Although the size and shape of the Mosaic may not exactly match the size and shape of the specified area, the entire specified area is always included in the captured images.

Once the Mosaic is captured and displayed, you can zoom in on any part of it and draw a map anywhere on it. You can also save the Mosaic in a file that can be opened later using a program that opens bitmap files, copy it to the Windows Clipboard for pasting into a document, or print it on paper. See “Saving a Mosaic” “Copying a Mosaic” in this chapter and “Printing a Mosaic” in the “Printing” chapter for more information.

Note If the cross hairs that indicate the current stage location fall within the area of a Mosaic, the copy of the live video image in the navigation pane is replaced by the captured image of that sample area. If you move the stage so that the cross hairs are outside the Mosaic, the copy of the live video image once again appears in the navigation pane. ▲

You can clear, copy, save or print the Mosaic by using commands in the Atlμs menu and File menu. See the next sections and “Printing a Mosaic” in the “Printing” chapter for complete information.

Follow these steps to capture a Mosaic:

1. **Use the area map tool to draw a box in the navigation pane around the area of the sample for which you want a video record.**

   See "Drawing an area map (or Mosaic)" if you need help.

2. **Choose Capture Mosaic from the Atlμs menu.**

   The system captures video images of the specified area and displays them as a Mosaic in the navigation pane.

   To stop the capture process before completion, click the Stop button.

Tips Capturing a Mosaic

- Before you capture a Mosaic, make sure the current calibration is the correct calibration for the objective you are using. This ensures that the video images that make up the Mosaic appear well aligned, with their edges neatly connected. See "Opening a saved calibration" in the "Configuring the System" chapter or "Selecting a calibration" in this chapter for more information.

Clearing a Mosaic from the navigation pane

After you have used Capture Mosaic in the Atlμs menu to display a Mosaic, you can choose Clear Mosaic from the Atlμs menu to clear from the navigation pane all of the images except the image that matches the video pane. See "Capturing a Mosaic of video images for a sample area" for more information on displaying a Mosaic in the navigation pane.

Tips Clearing a Mosaic

- Be sure you want to clear the Mosaic before using this command. If you change your mind after clearing the images, you will have to capture all of them again to restore the Mosaic.

Copying a Mosaic

After you have used Capture Mosaic in the Atlμs menu to display a Mosaic, you can choose Copy Mosaic from the Atlμs menu to copy the Mosaic, along with the navigation pane axes, to the Windows Clipboard. You can then paste the Mosaic into a document using a word processing program or other program that lets you paste items from the Clipboard. See "Capturing a Mosaic of video images for a sample area" for more information on displaying a Mosaic in the navigation pane.

Saving a Mosaic

After you have used Capture Mosaic in the Atlμs menu to display a Mosaic, you can use Save Mosaic in the Atlμs menu to save the Mosaic, along with the navigation pane axes, in a bitmap file. You can then open the file using a program that opens bitmaps. See "Capturing a Mosaic of video images for a sample area" for more information on displaying a Mosaic in the navigation pane.

Follow these steps to save a Mosaic:

1. **Choose Save Mosaic from the Atlμs menu.**

   The Save As dialog box appears.

2. **Type a file name in the File Name text box.**

3. **Locate and open the directory where you want the Mosaic saved.**

4. **Choose Save.**

Setting the automated Reflex aperture

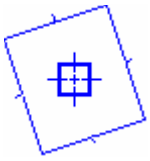
The next sections explain three ways to set the automated Reflex aperture system on a Continuμm microscope. You can also set the aperture by using the Aperture button on the Mapping tab of the Experiment Setup dialog box. See "Specifying the automated Reflex aperture" for details.

Important Use only the software to adjust the aperture; do *not* use the Reflex aperture control knobs on the microscope. If you do adjust the knobs, you will need to initialize the aperture. See "Initializing the automated Reflex aperture" in the "Configuring the System" chapter for instructions. ▲

For more information about the Reflex aperture, see the documentation that came with your microscope.

Adjusting the automated Reflex aperture graphically

If you have a Continuμm microscope with the automated Reflex aperture, the aperture is represented in the video pane of the Atlμs window by a box you can manipulate. Here is an example:



Use the arrow tool to change the size, shape and orientation of the box. Simply select the tool and then drag a side or corner of the box. The Reflex aperture is adjusted automatically to match the box.

Since the box is always present, the aperture tool is not available.

Note The minimum size of the automated Reflex aperture is nominally 5 by 5 micrometers. If you attempt to set the aperture to this or a smaller size, the system will automatically adjust the aperture to the minimum size possible on your microscope (typically 8 by 8 micrometers). The minimum available size varies slightly from system to system. ▲

Your graphical adjustment of the aperture changes in the settings in the dialog boxes displayed by Aperture Dimensions in the Atlμs menu (see the next section) and the Aperture button on the Mapping tab of the Experiment Setup dialog box. See "Specifying the automated Reflex aperture" for details.

Setting the automated Reflex aperture numerically

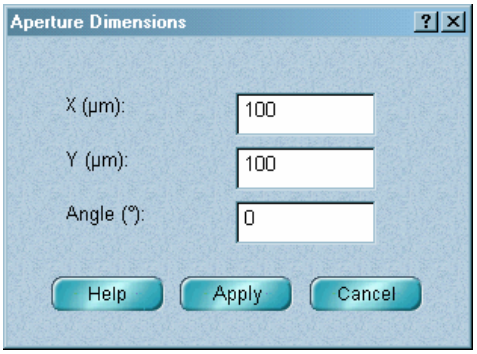
You can use Aperture Dimensions in the Atlμs menu to adjust the size, shape and orientation of the automated Reflex aperture by entering numerical values.

Note The minimum size of the automated Reflex aperture is nominally 5 by 5 micrometers. If you attempt to set the aperture to this or a smaller size, the system will automatically adjust the aperture to the minimum size possible on your microscope (typically 8 by 8 micrometers). The minimum available size varies slightly from system to system. ▲

Follow these steps to set the automated Reflex aperture numerically:

1. **Choose Aperture Dimensions from the Atlμs menu.**

   The Aperture Dimensions dialog box appears:



The settings in this dialog box are linked to those in the dialog box displayed by the Aperture button on the Mapping tab of the Experiment Setup dialog box. See "Specifying an aperture" for more information.

2. **Type the X dimension of the aperture in micrometers, before any rotation, in the X (µm) text box.**

3. **Type the Y dimension of the aperture in micrometers, before any rotation, in the Y (µm) text box.**

4. **Specify the angle by which to rotate the aperture about the center of the field of view within the plane of the sample.**

   To do this, type a number in the Angle (degrees) text box. An angle of 0 positions the aperture with its X dimension parallel to the X-axis. You can rotate the aperture from 45 to -45 degrees (a negative angle rotates the aperture clockwise). With this range of rotation plus the ability to resize the aperture, any combination of orientation and rectangular shape is possible.

5. **Choose Apply.**

   The aperture is adjusted according to your settings. You can view the sample and make further adjustments if desired.

6. **When you are finished, choose Close.**

Setting the automated Reflex aperture to the default

Choose Set Aperture To Default from the Atlμs menu to set the automated Reflex aperture to the default size and zero degrees of rotation. If you are using an objective with a magnification of 15X or less, the default size is 100 by 100 micrometers. If you are using an objective with a magnification greater than 15X, the default size is 50 by 50 micrometers.

Note The software bases the default aperture on the setting of the Objective parameter that was saved in the current calibration. ▲

Setting the FT-Raman View Stage origin

Before you use OMNIC Atlμs with an FT-Raman View Stage, use Move Stage in the Atlμs menu to establish the specified center of horizontal stage travel as the zero (0,0) point. The zero point will be used as a reference for the X and Y values of sample points you specify, maps and annotation you draw, and axes displayed in the Atlμs window.

Note Before you use the FT-Raman View Stage, it must be initialized so that the stage coordinate values displayed by the software are repeatable and accurate with respect to the laser location. First make sure the stage cable is connected to the connecter on the rear wall of the sample compartment and then start OMNIC For Raman. When the OMNIC For Raman window appears, the stage has been initialized. ▲

Follow these steps:

1. **Place the sample cup in the hole in the stage.**

2. **Move the stage to position the sample cup in the field of view.**

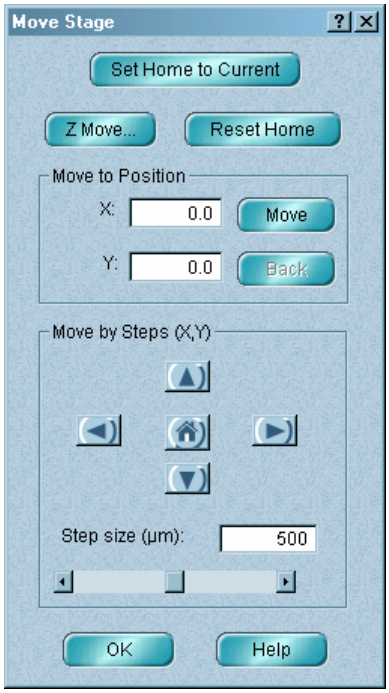
   You can use the stage movement tool or Move Stage in the Stage menu to do this.

3. **Focus on the inside bottom surface of the cup.**

   You should see machined concentric circles on the surface.

4. **Choose Move Stage from the Atlµs menu.**

   The Move Stage dialog box appears:



5. **Use the arrow buttons in the Move By Steps (X,Y) box to move the stage to center the concentric circles on the cross hairs.**

   You may need to drag the dialog box out of the way first.

   See “Moving the stage with the Move Stage command” in the “Preparing for Data Collection” chapter if you need help using the buttons.

6. **Choose OK.**

   The center of the cup is now at the origin point (0,0).

Collecting Data

After you have set up data collection as explained in the preceding chapter, follow the instructions in this chapter to collect a map or individual spectra.

Collecting a map background

Collect Map Background, if available in the Collect menu, lets you collect a background at the specified background point. Often a background is collected as part of the infrared mapping experiment, and there is no need to use Collect Map Background. See "Specifying a background point" and "Background handling" in the "Preparing for Data Collection" chapter for information about specifying a background point and when to collect a background. See "Collecting an FT-IR or FT-Raman map" in this chapter for complete information on collecting map data.

Note You can also collect a background at the current stage location, as explained in the next section. ▲

There does not need to be a current map sequence in order to collect the background. This lets you collect a background on a sample you are going to map or on another sample, before collecting the map.

See "Collecting backgrounds for FT-IR experiments" in the "Overview" chapter for information on deciding how to collect a background.

Note If you want the collected background to be used for a map you plan to specify, delete the background point before collecting the map. Otherwise, another background will be collected (using the sample) when you collect the map. See "Deleting a background point" in the "Preparing for Data Collection" chapter for information on deleting a background point. ▲

Follow these steps to collect a background with Collect Map Background:

1. **Prepare for background collection.**

   Install the appropriate material on the stage and specify a background point. Install the aperture if desired (and flip the microscope mirrors if they are not automated).

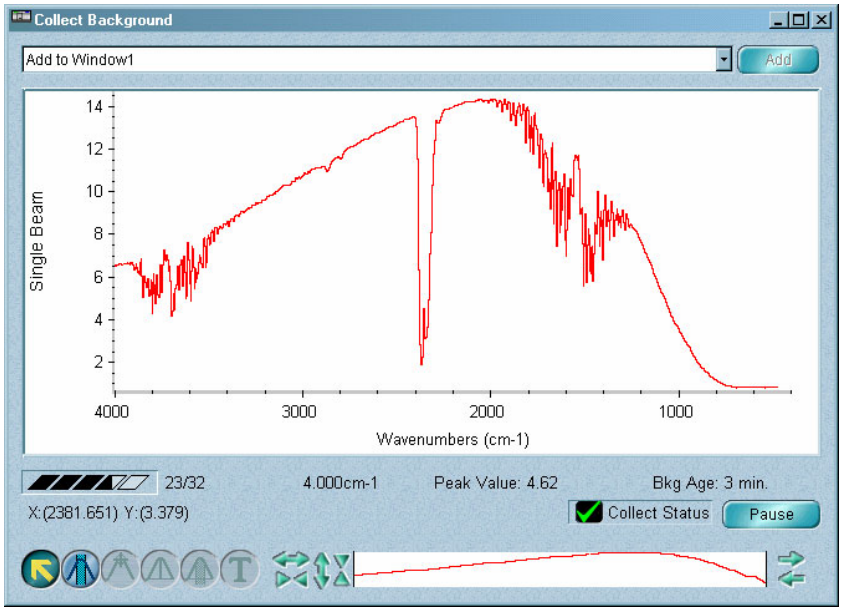
   If you are collecting ATR data, you need to collect the data through the clean ATR crystal. See the documentation that came with your ATR crystal for more information.

2. **Choose Collect Map Background from the Collect menu, and then follow the instructions that appear on the screen.**

   If the following prompt appears, make sure the system is prepared to collect the background and then choose OK.

This prompt appears if Prompt To Insert Or Remove Sample is selected on the Collect tab of the Options dialog box, available through Options in the Edit menu.

During collection the data appears in the Collect Background window. Here is an example:



The status of the collection appears in the description bar. For more information about using this window, choose OMNIC Help Topics from the Help menu, find "background spectrum" in the Index and go to the "Collecting a background spectrum" topic.

If data collection is finished and the Collect Background window is displayed, you can move the spectrum to a spectral window by selecting the desired option from the window selection box at the top of the window and then choosing Add. If you don't want to add the spectrum to a spectral window, close the Collect Background window by clicking the Close button (labeled "X") in the upper-right corner.

If a message asks whether to add the spectrum to a window, choose OK to add the background spectrum to a spectral window, or choose Cancel to return to the Collect Background window. To view information about collection problems, choose View Collect Status in the message.

➨ *Tips* ➨ Collecting a background

Collect the background using an area where there is no sample material present. The best location or material to use for collecting a background varies depending on the sample type or application. The table below provides some suggestions for collecting backgrounds.

Sample Type/Application	Background
transmission; sample suspended over air	Air.
transmission; sample on a salt plate	An area of the salt plate where no sample material is present.
transmission; sample in a compression cell	A crystal of KBr (or other halide salt) in the same compression cell, next to the sample.
specular reflection	A mirror or polished metal.
diffuse reflection	Crushed KBr, silicon carbide paper or other rough, non-infrared-absorbing material.
reflection-absorption	A mirror or polished metal, or an area of the sample support where no sample material is present.

Sample Type/Application	Background
grazing angle reflection	A mirror or polished metal, or an area of the sample support where no sample material is present.
ATR	Air.

Collecting a background spectrum at the current stage location

Use Collect Background, if available in the Collect menu, as explained below to collect a background at the current stage location. There is no need to use a tool to specify a background point; the spectrum will be collected at the current X,Y location. The collected background becomes the current background and will be used to ratio the sample spectra you collect until a new background is collected. In OMNIC Help Topics find "background spectrum" in the Index and go to "Collecting a background spectrum" for detailed instructions.

1. **Prepare for background collection.**

   Use Experiment Setup in the Collect menu to set Sample Compartment on the Bench tab for the location of the microscope and the type of collection you are performing. For more information, choose OMNIC Help Topics from the Help menu, find "sample compartment" in the Index and go to the "Specifying the sample location" topic.

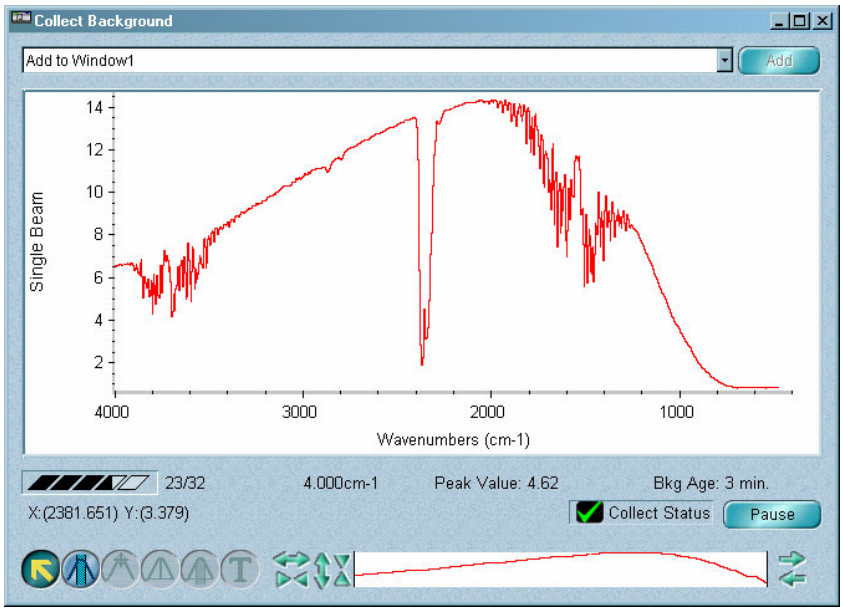
   Set Final Format on the Collect tab to the format that is appropriate for the kind of data you will be collecting.

   Install the aperture if desired (and flip the microscope mirrors if they are not automated).

   If you are collecting ATR data, you need to collect the data through the clean ATR crystal. See the documentation that came with your ATR crystal for more information.

2. **Choose Collect Background from the Collect menu, and then follow the instructions that appear on the screen.**

During collection the data appears in the Collect Background window. Here is an example:



The status of the collection appears in the description bar. For more information about using this window, choose OMNIC Help Topics from the Help menu, find “background spectrum” in the Index and go to the “Collecting a background spectrum” topic.

If a message asks whether to add the spectrum to a spectral window, choose Yes to add the background spectrum to the indicated window; choose No to end the procedure without saving the spectrum; or choose More Scans to return to the Collect Background window. To view information about collection problems, choose View Collect Status in the message.

If data collection is finished and the Collect Background window is displayed, you can move the spectrum to a spectral window by selecting the desired option from the window selection box at the top of the window and then choosing Add. If you don’t want to add the spectrum to a spectral window, close the Collect Background window by clicking the Close button (labeled “X”) in the upper-right corner.

Collecting an FT-IR or FT-Raman map

Follow the steps below to use Collect Map in the Collect menu to collect an FT-IR or FT-Raman map defined by a map sequence. See "Collecting a visible Raman map" if you have a Nicolet Almega system.

Note For this procedure the software has been set up to use the same sample for the background and sample spectra. Also, the software prompts you to prepare for data collection. By setting features described in "Setting the mapping options" and "Setting the data collection parameters for FT-IR and FT-Raman experiments" in the "Preparing for Data Collection" chapter, you can alter the order of some steps and make other changes to better fit your application. For example, you can specify a stored background or use a different material for the background. ▲

1. **Install the sample on the microscope stage.**

2. **Specify the map sequence or open a stored experiment file or sequence file.**

   See "Specifying a map sequence" in the "Preparing for Data Collection" chapter if you need help.

3. **Use Experiment Setup in the Collect menu to check or set the data collection parameters.**

   Select the appropriate Background Handling option on the Collect tab of the Experiment Setup dialog box. See "Background handling" in the "Preparing for Data Collection" chapter for details.

   Set Final Format on the Collect tab to the format that is appropriate for the kind of data you will be collecting.

   Set Sample Compartment on the Bench tab for the location of the microscope and the type of experiment you are performing. For more information, choose OMNIC Help Topics from the Help menu, find "sample compartment" in the Index and go to the "Specifying the sample location" topic.

   If you have a Continuμm XL microscope and are performing an imaging experiment, set Detector on the Bench tab to XL Array.

4. **If you are collecting a line map or area map, specify the profile type if desired.**

   You can use the Mapping tab of the Experiment Setup dialog box in the Collect menu to specify the profile type and associated information such as peak locations, spectral regions or baselines. See "Setting the Profile parameters" in the "Preparing for Data Collection" chapter for complete information.

   If you don't specify a profile type, the default profile will be used: Chemigram. This shows the integrated spectral intensity of a specified spectral region for each sample point.

5. **If you selected Save Video Frames In Map File in the Options dialog box (available through the Collect button on the Mapping tab of the Experiment Setup dialog box), remove the aperture from the microscope.**

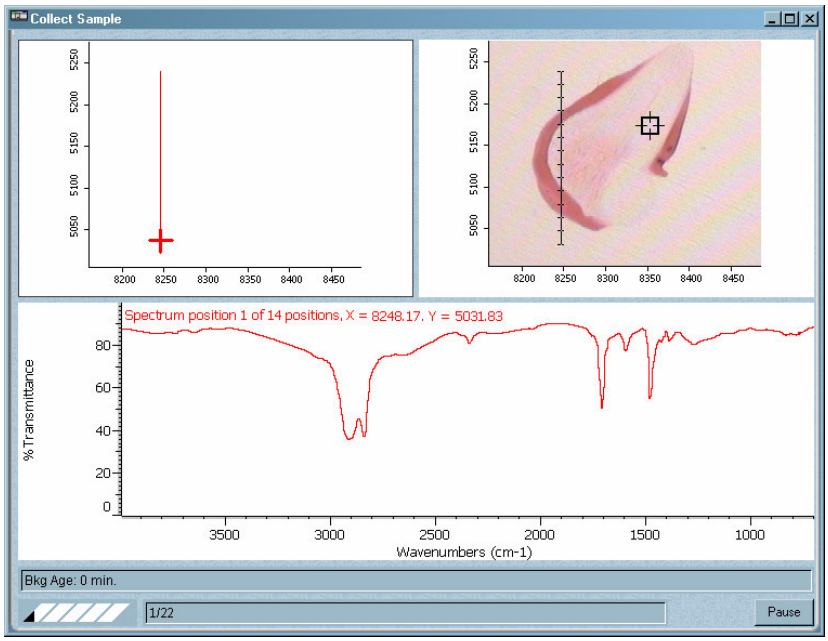
Note If you have a Continuμm microscope, the aperture cannot be removed. Instead, turn off the Reflex aperture illuminator to cause the aperture image to disappear. ▲

6. **Choose Collect Map from the Collect menu.**

   The Save As dialog box appears.

7. **Specify a file name and location for the map and then choose Save. Follow the instructions that appear on the screen.**

   The Collect Sample window appears and map data collection begins. Here is an example:



Collect Sample window

The description bar shows the progress of the collection. Cross hairs move to each sample point in the navigation pane as the corresponding spectrum is collected. The collected spectra appear in the spectral display pane.

If a prompt asks you to prepare to capture the video images, remove the aperture from the microscope if it is not already removed (if you have a Continuμm microscope, see the Note in step 5). Then choose OK. The images are captured and saved.

If a prompt asks you to prepare for map data collection, install the aperture (and flip the microscope mirrors if they are not automated) and then choose OK.

Note If you have a Continuμm microscope, adjust the aperture as desired. ▲

If Preview Data Collection is selected on the Collect tab of the Experiment Setup dialog box, preliminary data collection begins and the data are displayed in the Collect Sample window. If you are satisfied with the data, start the actual sample data collection by clicking the Start Collection button. If you don't want to collect a sample spectrum, click the Stop button to end the procedure.

Note If you are collecting ATR data, you need to make contact with the sample. See the documentation that came with your ATR crystal for more information. If you have the required hardware, you can use ATR mode or auto ATR contact to make and release contact with the sample automatically during data collection. See "Collecting ATR data with autofocus" or "Using auto ATR contact" for details. ▲

To stop data collection, click the Stop button.

You can pause data collection by clicking the Pause button. This lets you refocus the microscope or make contact with an ATR sample.

When the collection is finished, the data appears in a map window.

If any errors occurred during data collection, a window appears listing the errors in chronological order. Close the window after you read the error descriptions.

Collecting a visible Raman map

Follow the steps below to use Collect Map in the Collect menu to collect a visible Raman map defined by a map sequence. See the next section for information about collecting a depth profile. See "Collecting an FT-IR or FT-Raman map" if you have an FT-IR or FT-Raman system.

Note By setting features described in "Setting the mapping options" and "Setting the data collection parameters for visible Raman experiments" in the "Preparing for Data Collection" chapter, you can alter the order of some steps and make other changes to better fit your application. ▲

1. **Install the sample on the microscope stage.**

2. **Specify the map sequence or open a stored experiment file or sequence file.**

   See "Specifying a map sequence" in the "Preparing for Data Collection" chapter if you need help.

3. **Use Experiment Setup in the Collect menu to check or set the data collection parameters.**

   Select Microscope in the Beam Path/Sample Position box on the Bench tab. Set Final Format on the Collect tab to the format that is appropriate for the kind of data you will be collecting.

4. **If you are collecting a line map or area map, specify the profile type if desired.**

   You can use the Mapping tab of the Experiment Setup dialog box in the Collect menu to specify the profile type and associated information such as peak locations, spectral regions or baselines. See "Setting the Profile parameters" in the "Preparing for Data Collection" chapter for complete information.

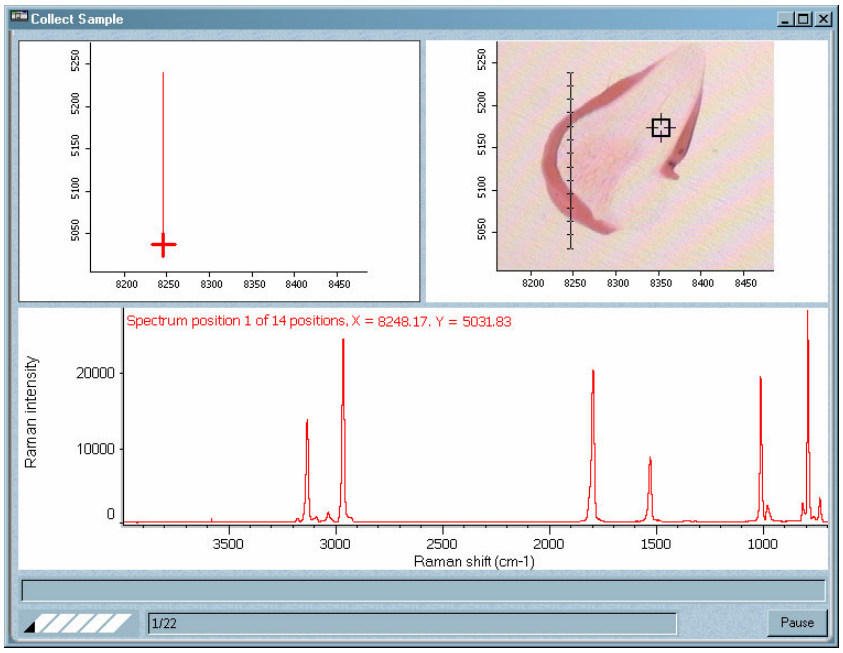
   If you don't specify a profile type, the default profile will be used: Chemigram. This shows the integrated spectral intensity of a specified spectral region for each sample point.

5. **Choose Collect Map from the Collect menu.**

   The Save As dialog box appears.

6. **Specify a file name and location for the map and then choose Save. Follow the instructions that appear on the screen.**

   The Collect Sample window appears and map data collection begins. Here is an example:



Collect Sample window

The description bar shows the progress of the collection. Cross hairs move to each sample point in the navigation pane as the corresponding spectrum is collected. The collected spectra appear in the spectral display pane.

If a prompt asks you to prepare to capture the video images, choose OK. The images are captured and saved.

If a prompt asks you to prepare for map data collection, choose OK.

If Preview Data Collection is selected on the Collect tab of the Experiment Setup dialog box, preliminary data collection begins and the data are displayed in the Collect Sample window. If you are satisfied with the data, start the actual sample data collection by clicking the Start Collection button. If you don't want to collect a sample spectrum, click the Stop button to end the procedure.

To stop data collection, click the Stop button.

You can pause data collection by clicking the Pause button. This lets you refocus the microscope.

When the collection is finished, the data appears in a map window.

If any errors occurred during data collection, a window appears listing the errors in chronological order. Close the window after you read the error descriptions.

To save the collected map, use Save Map or Save Map As in the File menu. See "Saving a map" in the "Saving and Exporting Map Data" chapter for details.

Collecting a depth profile

Follow the steps below to collect a line depth profile or area depth profile. See "Specifying the Dimensions parameters" in the "Preparing for Data Collection" chapter for more information about depth profiles.

1. **Place the sample on the microscope stage and focus at the desired depth.**

   You can focus above the sample surface, on the surface or below the surface. If you focus on the sample surface, you will be able to use the live display on the Bench tab of the Experiment Setup dialog box to maximize the signal in step 3.

2. **If you are collecting a line depth profile, use the sample point tool to click the desired location in the navigation pane or video pane. If you are collecting an area depth profile, use the line map tool to draw a line in either pane.**

3. **Use Experiment Setup in the Collect menu to set the data collection parameters.**

   On the Mapping tab of the Experiment Setup dialog box, select Depth Profile and then set the parameters, including the Z offset, if used. See "Specifying the Dimensions parameters" in the "Preparing for Data Collection" chapter for details.

   Choose OK to close the dialog box when you are finished.

4. **Choose Collect Map from the Collect menu.**

   The Save As dialog box appears.

5. **Specify a file name and location for the map and then choose Save. Follow the instructions that appear on the screen.**

   The Collect Sample window appears and map data collection begins. See the preceding section for a discussion of the window and the prompts that may appear.

   To save the collected depth profile, use Save Map or Save Map As in the File menu. See "Saving a map" in the "Saving and Exporting Map Data" chapter for details.

Collecting a sample spectrum at the current stage location

The following sections explain how to collect a sample spectrum at the current stage location on FT-IR, FT-Raman and visible Raman systems.

Collecting an FT-IR or FT-Raman spectrum at the current stage location

Use Collect Sample (or Collect Raman if you are using Raman hardware) in the Collect menu as explained below to collect a sample spectrum at the current stage location. There is no need to use a tool to specify a sample point; the spectrum will be collected at the current X,Y location. In OMNIC Help Topics find "sample spectrum" in the Index and go to "Collecting a sample spectrum" for detailed instructions. (In Raman Help Topics, find "Raman spectrum" in the Index and go to the "Collecting a Raman spectrum" topic.)

1. **Set the data collection parameters.**

   Use Experiment Setup in the Collect menu to set Sample Compartment on the Bench tab for the location of the microscope and the type of collection you are performing. For more information, choose OMNIC Help Topics from the Help menu, find "sample compartment" in the Index and go to the "Specifying the sample location" topic. (If you are collecting Raman data, find "beam path" in the Index of Raman Help Topics and go to the "Specifying the beam path" topic.)

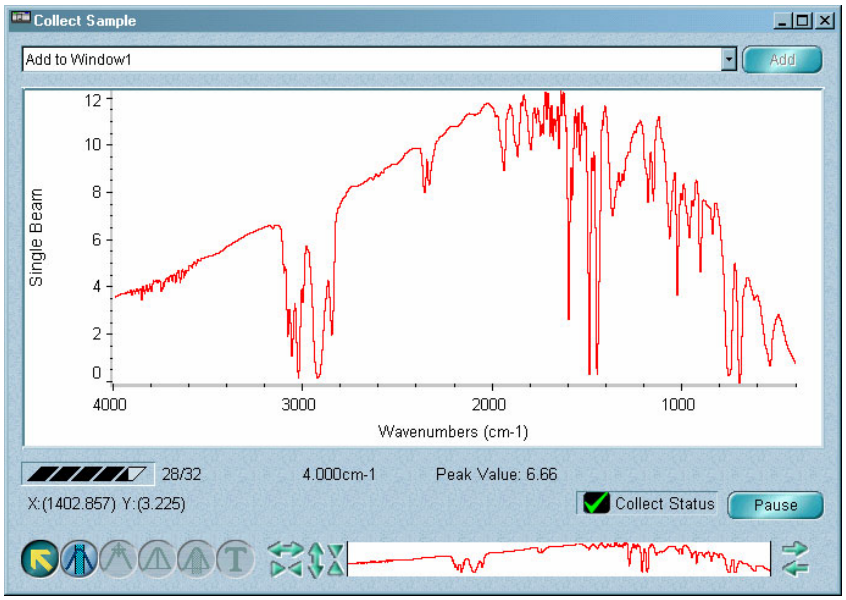
   Set Final Format on the Collect tab to the format that is appropriate for the kind of data you will be collecting.

   Install the aperture if desired (and flip the microscope mirrors if they are not automated).

2. **Choose Collect Sample (or Collect Raman) from the Collect menu, and then follow the instructions that appear on the screen.**

Note If you are collecting ATR data, you need to make contact with the sample. See the documentation that came with your ATR crystal for more information. If you have the required hardware, you can use ATR mode or auto ATR contact to make and release contact with the sample automatically during data collection. See "Collecting ATR data with autofocus" or "Using auto ATR contact" for details. ▲

During collection the data appears in the Collect Sample (or Collect Raman) window. Here is an example:



The status of the collection appears in the description bar. For more information about using this window, choose OMNIC Help Topics from the Help menu, find “sample spectrum” in the Index and go to the “Collecting a sample spectrum” topic. (If you are collecting Raman data, find “Raman spectrum” in the Index of Raman Help Topics and go to the “Collecting a Raman spectrum” topic.)

If data collection is finished and the Collect Sample (or Collect Raman) window is displayed, you can move the spectrum to a spectral window by selecting the desired option from the window selection box at the top of the window and then choosing Add. If you don’t want to add the spectrum to a spectral window, close the Collect Sample (or Collect Raman) window by clicking the Close button (labeled “X”) in the upper-right corner.

If a message asks whether to add the spectrum to a spectral window, choose Yes to add the spectrum to the indicated window; choose No to end the procedure without saving the spectrum; or choose More Scans to return to the Collect Sample (or Collect Raman) window. To view information about collection problems, choose View Collect Status in the message.

Collecting a visible Raman spectrum at the current stage location

Use Collect Sample in the Collect menu as explained below to collect a sample spectrum at the current stage location. There is no need to use a tool to specify a sample point; the spectrum will be collected at the current X,Y location. In OMNIC Help Topics find "Collect Sample command" in the Index and go to "Collecting a sample spectrum" for detailed instructions.

1. **Set the data collection parameters.**

   Use Experiment Setup in the Collect menu to select Microscope in the Beam Path/Sample Position box on the Bench tab.

   Set Final Format on the Collect tab to the format that is appropriate for the kind of data you will be collecting.

2. **Choose Collect Sample from the Collect menu, and then follow the instructions that appear on the screen.**

   During collection the data appears in the Collect Sample window. The status of the collection appears in the description bar.

   If data collection is finished and the Collect Sample window is displayed, you can move the spectrum to a spectral window by selecting the desired option from the window selection box at the top of the window and then choosing Add. If you don't want to add the spectrum to a spectral window, close the Collect Sample window by clicking the Close button (labeled "X") in the upper-right corner.

   If a message asks whether to add the spectrum to a spectral window, choose Yes to add the spectrum to the indicated window; choose No to end the procedure without saving the spectrum; or choose More Scans to return to the Collect Sample window. To view information about collection problems, choose View Collect Status in the message.

Collecting ATR data with autofocus

If you have an FT-IR system with the optional autofocus feature, you can use ATR mode to break and restore contact with the sample automatically during an experiment.

Important Always lower the stage to break contact with the ATR crystal before moving the stage in the X or Y directions. Use the Z Position button to lower the stage. ▲

Note If you have a Continuμm XL microscope, do not use the linear array detector for ATR experiments. ▲

To use ATR mode with a ZnSe or diamond crystal:

1. **Specify the X and Y coordinates of the sample points just as you would for any mapping experiment.**

2. **With the microscope in View mode and ATR objective in position, carefully raise the stage with the Z Position button (shown below) to make contact with the sample.**

   There will be a wetting effect or slight darkening of the field. See the documentation that came with your ATR crystal for more information.

3. **Click the Store Z Position button (shown below) to save the Z coordinate of the stage position.**

   This coordinate will be used to make contact at every sample point in the experiment.

4. **Start data collection.**

To use ATR mode with any type of crystal:

1. **Specify the X and Y coordinates of the sample points just as you would for any mapping experiment.**

2. **With the microscope in infrared mode, the ATR objective in position, and the single-beam spectrum displayed in the Experiment Setup dialog box, carefully raise the stage using the autofocus hardware controller to make contact with the sample.**

   You should be able to see the sample absorption bands in the single-beam spectrum.

3. **Click the Store Z Position button (shown below) to save the Z coordinate of the stage position.**

   This coordinate will be used to make contact at every sample point in the experiment.

4. **Start data collection.**

Using auto ATR contact

If you have a Continuµm microscope with the optional auto ATR contact feature, you can collect ATR spectra with the optimal contact pressure automatically applied by the system.

Note If you have a Continuµm XL microscope, do not use the linear array detector for ATR experiments. ▲

- If you are collecting an individual spectrum at the current stage location, use the ATR Contact button (shown below) to establish optimal contact with the sample.

  The button uses the microscope's internal Contact Alert System to determine the optimal contact. See the procedure later in this section for details.

  After contact is made, the ATR Contact button changes appearance:

  Use the button to release contact.

- If you are collecting a map, select Auto ATR Contact in the Focus dialog box (available through the Focus button on the Mapping tab of the Experiment Setup dialog box) before starting the collection. With this option selected, the system automatically makes and releases contact with the sample at each sample point (the ATR Contact button is not used), but not at the background point. Because this feature uses the internal Contact Alert System instead of a single stored Z value to make sample contact, you can automatically collect a map of a sample of varying thickness without damaging the crystal or objective. See the procedure later in this section for details.

Note When OMNIC Atlμs starts, it checks to see if the Z-axis of the microscope has been initialized. If the axis has not been initialized, you are asked whether to initialize it.

- If you cancel the initialization, the autofocus and auto ATR contact features are disabled until the next time you start OMNIC Atlμs.
- If you initialize the Z-axis, the stage moves to its upper and lower limits and then back to the origin. After initialization, the stage returns to its former position. ▲

Important Lower the condenser all the way and remove the nosepiece from the microscope before initialization. ▲

To collect an ATR spectrum automatically:

1. **Set up the internal Contact Alert System.**

   See the documentation that came with your microscope for instructions.

2. **Install the sample and position the area of interest under the ATR objective or slide-on ATR attachment.**

3. **Click the ATR Contact button (shown below).**

   The stage automatically moves upward to make optimal contact with the sample. While the stage is moving upward, the button is labeled "Abort." If for any reason you need to stop the stage, click the button.

   After contact is made, the ATR Contact button changes appearance and is used to release contact:

Important You can use the Z Position button (shown below) to adjust the contact pressure.

However, be careful when moving the stage up, since applying too much pressure can damage the ATR objective or crystal! Choose Experiment Setup from the Collect menu, and watch the live single-beam spectrum on the Bench tab for the appearance of sample absorptions to determine when optimal pressure has been achieved. ▲

Note If you use the Z Position button to change the contact pressure, the ATR Contact button's appearance and use (described above) will depend on the current pressure. If you use the Z Position button to move the stage upward, the computer will beep and the software will warn you about the risk of damage to the objective, sample or crystal. ▲

4. **Choose Collect Sample from the Collect menu.**

5. **When data collection is finished, click the ATR Contact button to release contact.**

   The stage moves downward to release contact with the sample.

To collect an ATR map automatically:

1. **Set up the internal Contact Alert System.**

   See the documentation that came with your microscope for instructions.

2. **Install the sample and position the area of interest under the ATR objective or slide-on ATR attachment.**

3. **Specify the map sequence.**

   Use the Atlμs window tool palette or the Mapping tab of the Experiment Setup dialog box to do this.

   Be sure to select Auto ATR Contact in the Focus dialog box (available through the Focus button on the Mapping tab).

4. **Choose Collect Map from the Collect menu.**

   The system automatically makes and releases contact with the sample at each sample point while collecting the map.

Opening and Importing Map Data

This chapter explains how to open and import map data stored on a disk.

Opening a map or files from a split map

Use Open in the File menu to open a collected map, a depth profile, principal component analysis (PCA) results, Multivariate Curve Resolution (MCR) results or quantitative analysis results that were previously saved with Save Map or Save Map As in the File menu. (See "Saving a map" or "Saving a map with a new file name or in a different location" in the "Saving and Exporting Map Data" chapter for more information.) You can also open multiple .CSV or .JDX (JCAMP-DX) files that were saved when you split a map and display them in a spectral window. (See "Splitting a map into separate data files" in the "Processing and Analyzing Map Data" chapter for more information.)

After you open a map, you can view and manipulate the map data. See "Performing a principal component analysis" in the "Processing and Analyzing Map Data" chapter for information about principal component analyses. See "Using Multivariate Curve Resolution" in that chapter for information about MCR analyses. See "Quantifying a map" in that chapter for information about performing a quantitative analysis.

Note You can also display a map by importing an ENVI®, JCAMP-DX or spectral group file with Import in the File menu as explained in the next section. ▲

Follow the steps below to open a map, a depth profile, PCA results, MCR results or quant results.

For information about opening multiple .CSV or .JDX files, choose OMNIC Help Topics from the Help menu, find "CSV file format" in the Index and go to the "Opening a CSV text file" topic. The provided instructions apply to both .CSV and .JDX files.

1. **Choose Open from the File menu.**

   The Open dialog box appears.

2. **Set Files Of Type to Mapping Files (*.MAP).**

3. **Type the name of the file you want to open in the File Name text box, or locate and select a file.**

4. **Choose Open.**

   The map appears in a new map window. See “Using map windows” in the “Displaying Map Data” chapter for more information.

   A special window is used to display opened PCA results or MCR results. See “Performing a principal component analysis” or “Using Multivariate Curve Resolution” in the “Processing and Analyzing Map Data” chapter for details.

Note Some commands in the Process menu let you save both the original and processed spectra in the map file. If both are present in the file you are opening, a prompt asks you which spectra to open. Respond appropriately. ▲

Importing map data

Use Import in the File menu to open an ENVI file, a spectral group file or multiple JCAMP-DX or CSV files and display the opened file or files as a map in a map window. Follow these steps:

1. **Choose Import from the File menu.**

   The Open dialog box appears.

2. **Set Files Of Type to the desired file type.**

3. **If you are importing a single file, type the name of the file or locate and select a file. If you are importing multiple JCAMP-DX or CSV files, locate and select the files.**

   You can change directories or drives to locate the file or files you want to open.

4. **Choose Open.**

   If you are importing a single file, the imported data appears in a new map window and the procedure is finished. See "Using map windows" in the "Displaying Map Data" chapter for more information.

   If you are opening multiple JCAMP-DX or CSV files, the Parameters dialog box appears showing information about the first file.

5. **Make any desired changes to the parameter settings and then choose OK or OK To All.**

   The parameter settings apply to all the files you are opening. You can click the More button to set additional parameters.

   The imported data appears in a new map window.

Displaying Map Data

OMNIC Atlμs uses map windows to display collected maps along with associated software features such as a video image of the sample and a 3-D display of the map data.

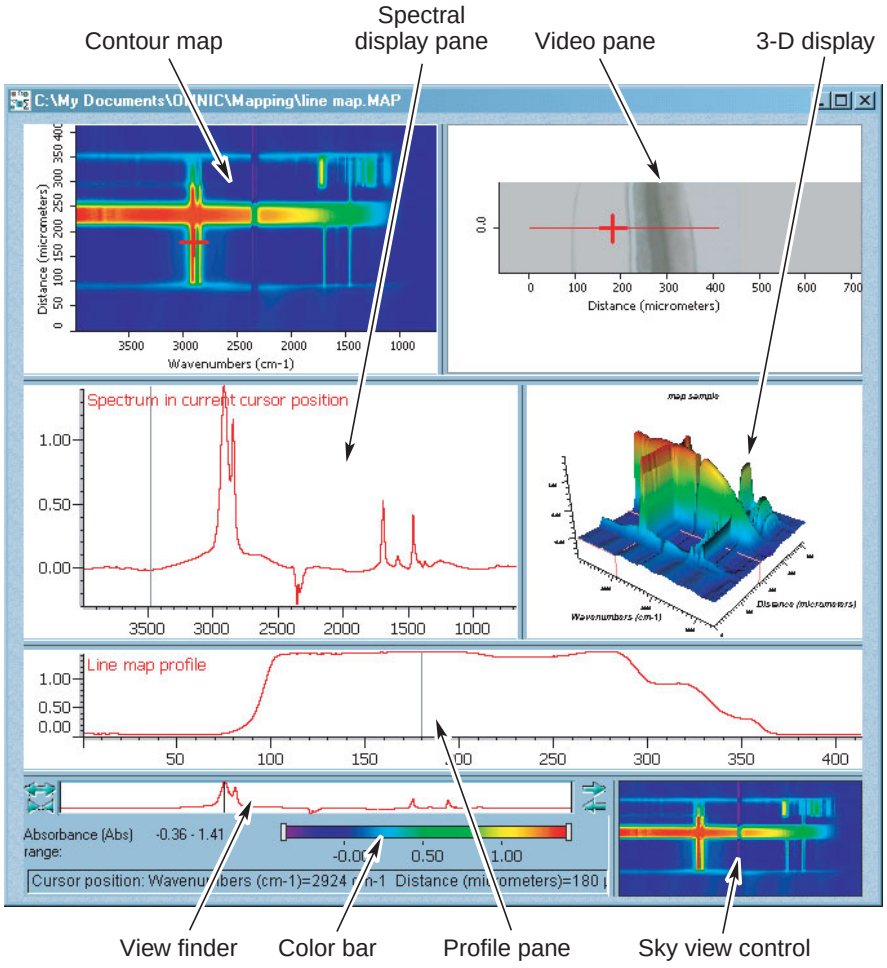
A separate map window is used for each map you display. After you collect a map or open a stored map, it is displayed in a new map window.

An important feature of a map window is the "interlinking" of the video image, the contour map (or discrete point location map), 3-D display and other parts of the window. This lets you see the relationship between data displayed in different ways.

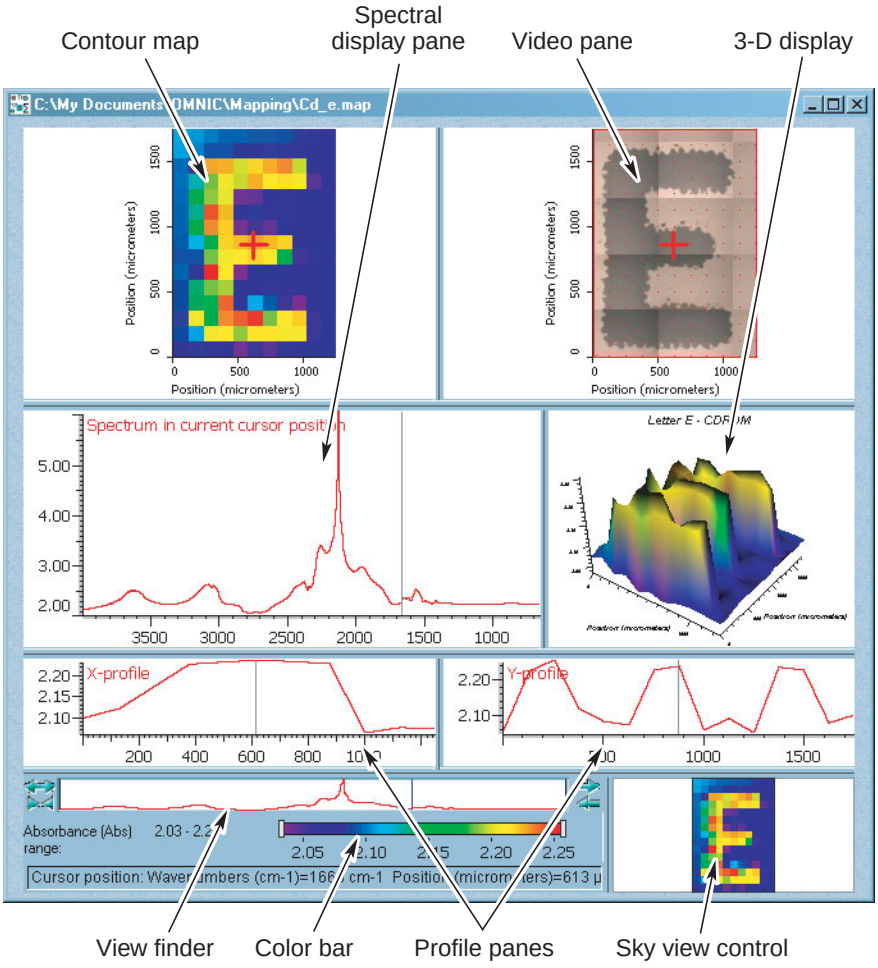
Using map windows

You can display a line map, area map, discrete point map or depth profile in a map window. The features provided in the window for viewing and manipulating map data depend on the options selected on the Mapping - General tab of the Display Setup dialog box. (See "Specifying the items to display" for more information.) The displayed features can include some or all of the items shown in the following illustrations. The features used to display a depth profile are the same as those for displaying a line map or area map. The window features work the same for any data type.

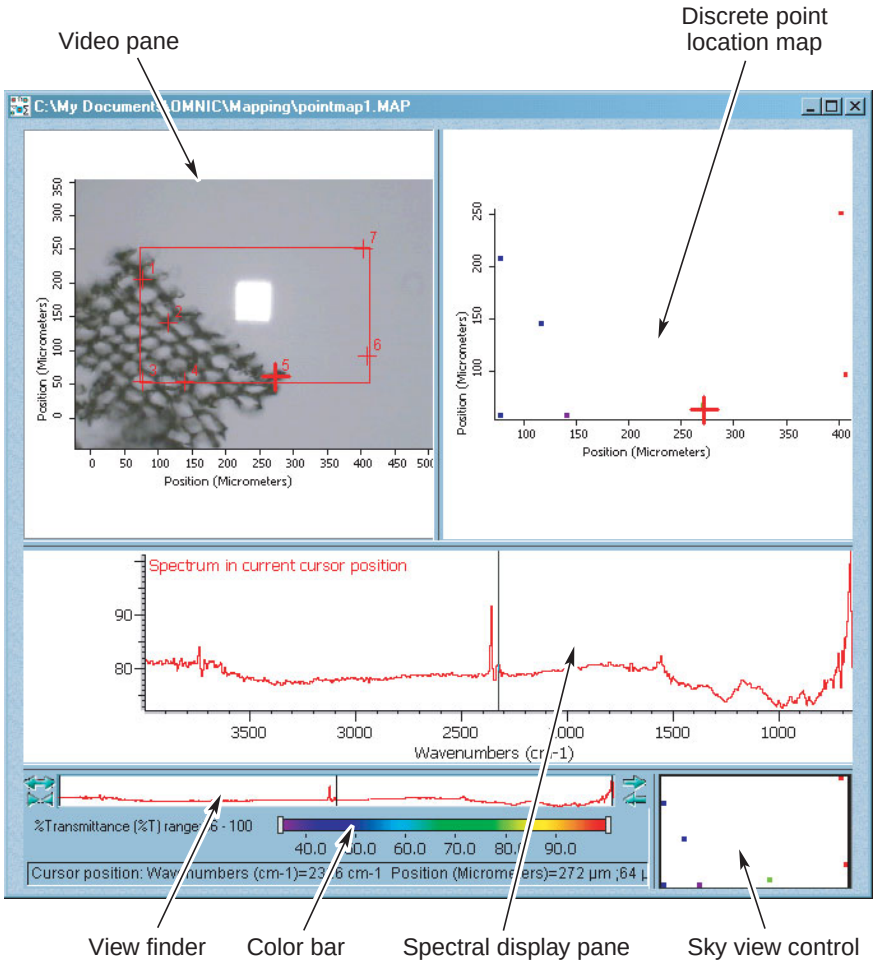
Note Profile windows (created when you use Profile Setup or Show Current Profile in the Atlμs menu) are similar to map windows. In general the information in this section applies to both window types. ▲



Line map in a map window



Area map in a map window



Discrete point map in a map window

You can adjust the size and shape of the panes in the window by dragging their borders.

The view finder lets you adjust the displayed frequency range of the data. It works the same as the view finder in a spectral window, with the addition of the feature explained below. For more information choose OMNIC Help Topics from the Help menu, find “view finder” in the Index and go to the “View finder” topic.

The middle vertical line in the view finder lets you specify a frequency to use for displaying data in some of the panes. If you are displaying a line map, the specified frequency is used for the profile. If you are displaying an area map, the frequency is used for the 3-D image, the contour map (or discrete point location map) and the profiles. To change the frequency, drag the line to the right or left. (You can also use the Page Up and Page Down keys on the keyboard when the view finder is active.) As you move the line, the frequency range and the current frequency are displayed. The data in the affected panes changes to reflect the new frequency. (You can specify whether this change occurs as you move the line. See "Setting the spectral display parameters" for details.) You can animate this process for an area map by using Animation in the Atlμs menu. See "Animating your view of the map data" for instructions.

The color bar shows the colors used in the contour map (or discrete point location map) and 3-D image. The scale below the color bar indicates the values of the colors. The unit and range of available values appear to the left of the color bar. You can change the range by setting Minimum and Maximum in the Color Limits box on the Mapping - General tab of the Display Setup dialog box. See "Setting the color limits" for more information.

The vertical bars on the color bar indicate the limits of the value range currently used for the colors in the contour map and 3-D image. You can change this range by horizontally dragging the vertical bars. This in turn changes the distribution of the colors. You can also change the range by setting Background Threshold and Foreground Threshold on the Mapping - General tab of the Display Setup dialog box. See "Specifying the background and foreground thresholds" for more information.

If one or both of the vertical bars have been moved away from the ends of the color bar, you can drag the portion between the vertical bars to the left or right. To specify a different color scheme for the data, use the Color Scheme options on the Mapping - General tab of the Display Setup dialog box. See "Selecting a color scheme" for details.

You can copy the color bar to the Windows Clipboard by *right-clicking* the color bar and choosing Copy from the pop-up menu. You can then paste the image into a document using a program that pastes items from the Clipboard.

You can print the color bar by *right-clicking* it and choosing Print from the pop-up menu.

You can adjust the display limits for many of the items in the map window by using Display Limits in the View menu. See "Setting the display limits" for details.

The next sections explain how different kinds of map data are displayed in the panes of a map window.

To close the map window, click the Close button (labeled "X") in the upper-right corner.

Contour maps

If Contour Map is selected on the Mapping - General tab of the Display Setup dialog box, a contour map (or discrete point location map) appears in the map window or profile window. Contour maps (or discrete point location maps) use colors or lines to indicate ranges of value or the locations of equal value. The measured values can be spectral intensity or other types of value.

The spectrum most recently displayed in the spectral display pane (if present) corresponds to the cross hairs (or other cursor type) in the contour map (or discrete point location map). You can move the cross hairs by clicking a location in the map, dragging the cross hairs, or using the arrow keys on the keyboard when the map is active. The spectrum associated with the new location appears in the spectral display pane.

Note If a line icon or "T" appears next to the pointer, do the following before clicking a location or dragging the cross hairs: *Right-click* the contour map (or discrete point location map), point to Cursor Mode and choose Select And Zoom from the pop-up menu. ▲

Use the 2-D View tab of the Display Setup dialog box to change how the contour map (or discrete point location map) is displayed. See "2-D View display parameters" for details.

You can measure items in the contour map: *Right-click* the map, point to Cursor Mode, choose Ruler from the pop-up menu, and then drag across the map to draw a ruler. (The ruler also appears on the video image.) The measured distance appears near the lower-left corner of the map window. You can manipulate the ruler just as you would in the Atlμs window. See "Moving the ruler" and "Resizing the ruler" in the "Preparing for Data Collection" chapter if you need help. To remove the ruler, *right-click* the map, point to Cursor Mode and choose Select And Zoom from the pop-up menu.

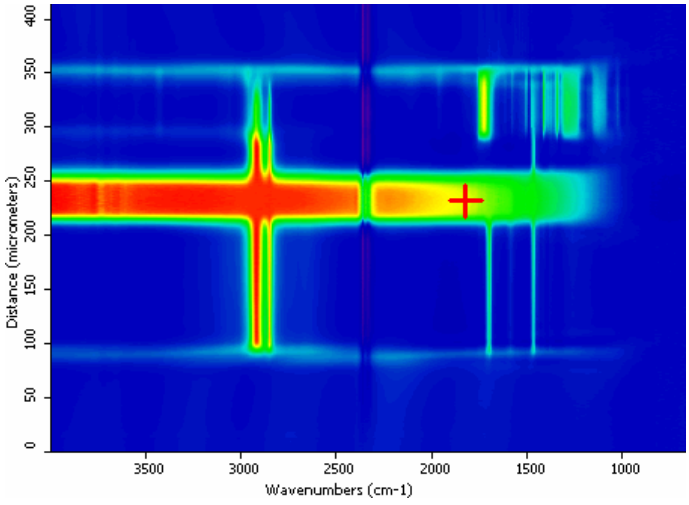
You can overlay the contour map (or discrete point location map) with the video image to see spatial relationships between the two. See "Overlaying the video image and contour map or discrete point location map" for details.

Read the next sections for more information about contour maps (and discrete point location maps).

Note You can remove the contour map (or discrete point location map) from the window by *right-clicking* it and then choosing Hide from the pop-up menu. ▲

Line and line depth profile contour maps

The following illustration shows a line contour map displayed in a map window. A contour map for a line depth profile would be similar.



Line contour map

A line or depth profile contour map is a graphical representation of the spectral intensity of the series of map spectra. Intensities can be indicated on the map in different ways. You can specify that "contours," areas of similar intensity displayed using the same color, be displayed with or without black outlines around them. You can also specify that colored lines be used instead to indicate intensities, as explained in "Setting the contour parameters."

To find the approximate intensity value of a contour or a colored line, locate the color on the color bar and read the value on the scale below the color bar.

To change how the colors are used to represent values, adjust the color bar by dragging the vertical white markers along the color bar. If one or both markers have been moved away from the ends of the color bar, you can move the pointer between the markers and then drag that segment of the color bar to the left or right. The changes you make to the color bar are reflected in the use of color in the contour map.

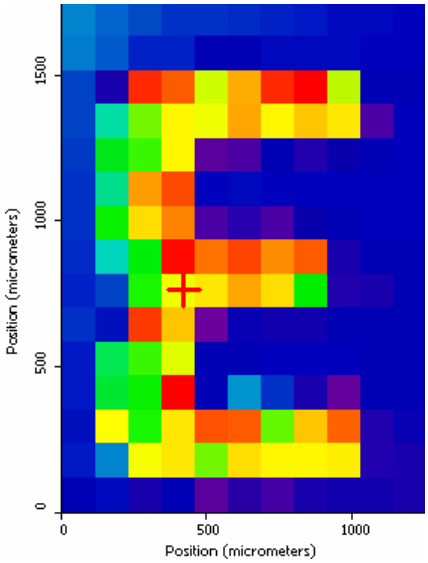
The X-axis of a line or line depth profile contour map is in wavenumbers or Raman-shifted wavenumbers and represents the frequencies at which spectral bands occur. The Y-axis is in micrometers and represents the distance from the first sample point at which each spectrum in the map was collected. (For a line depth profile, the axis represents the distance from the zero point.)

Note If you have a Nicolet Almega system and used a step size of less than 100 micrometers to collect the map, the Y-axis is in tenths of a micrometer (0.1 µm) instead of micrometers. ▲

Together, the contours and axes present a view of the map data in three dimensions: spectral intensity (shown by the colors or contour lines, or both) at different frequencies (indicated by the X-axis) at different distances on or within the sample from the starting point (indicated by the Y-axis). (If you create a profile from a line map or line depth profile, the result has two dimensions: spectral intensity and frequency.)

Area and area depth profile contour maps

The following illustration shows an area contour map displayed in a map window. A contour map for an area depth profile would be similar.



Area contour map

An area contour map is a graphical representation of values at a particular frequency at points in the map. Typically an area contour map indicates chemical composition at different locations on the sample. (See "Creating a profile" for a description of all the available profile types.) The current frequency is indicated by the location of the vertical line that is initially in the center of the view finder. You can change the frequency, as explained later in this section.

The values are indicated on the map by blended or banded colors or by lines, similar to how spectral intensities are represented in a line contour map. To determine the value represented by a color or adjust the color bar, follow the instructions given in the preceding section for line contour maps.

Note If you did not specify a profile type before collecting the map, the default type, Chemigram, is used for the initial area contour map, and the contour colors represent overall spectral intensity at the sample points. ▲

The X-axis of an area contour map is in micrometers and represents the X position (on the microscope stage) of the sample points where each map spectrum was collected. Similarly, the Y-axis of an area contour map is in micrometers and represents the Y position of the sample points.

The X-axis of an area depth profile contour map is in micrometers and represents the horizontal distance along the line drawn in the Atlμs window where each map spectrum was collected. Similarly, the Y-axis of an area depth profile contour map is in micrometers and represents vertical distance from the zero point.

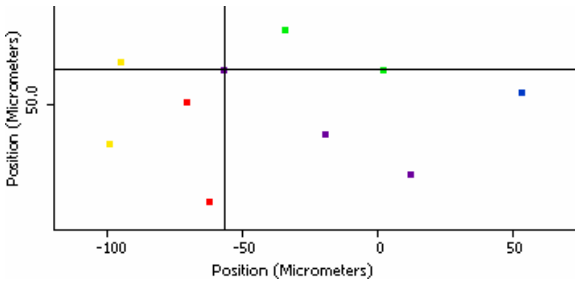
The scales of the axes are automatically adjusted so that the aspect ratio (proportions) of the contour map matches the mapped area in the video image. This makes it easy to identify corresponding locations in the contour map and video image.

Together, the colors of the contours or lines and the axes present a view of the map data at a particular frequency in three dimensions: value (shown by the colors) at different X positions (indicated by the X-axis) and different Y positions (indicated by the Y-axis).

Discrete point location maps

Here is an example of a discrete point location map displayed in a map window:

This type of map appears if you are displaying discrete point data and have selected Contour Map on the Mapping – General tab of the Display Setup dialog box.



Discrete point location map

A discrete point location map shows the locations of the sample points as well as their overall spectral intensities. To find the approximate intensity value of a point, locate its color on the color bar and read the value on the scale below the color bar. To adjust the color bar, follow the instructions given in the section called “Line and line depth profile contour maps.”

The X-axis of the location map is in micrometers and represents the X position (on the microscope stage) of the sample points where each map spectrum was collected. Similarly, the Y-axis of the location map is in micrometers and represents the Y position of the sample points.

Video pane

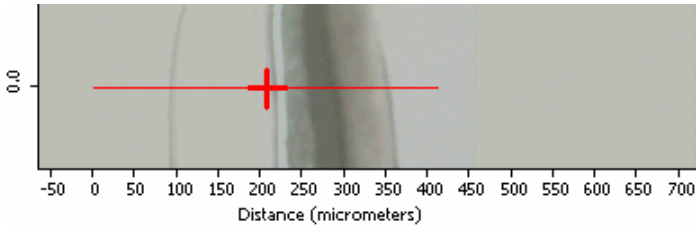
If Video Image is selected on the Mapping - General tab of the Display Setup dialog box, the map window or profile window contains the video image or Mosaic of video images of the sample surface that were captured during data collection. See "Capturing a Mosaic of video images for a sample area" in the "Preparing for Data Collection" chapter for information about capturing a Mosaic.

Note You can remove the video pane from the window by *right-clicking* it and then choosing Hide from the pop-up menu. ▲

The size of the sample area shown in the video image depends on which microscope objective was used to view the sample and save video images. If you want the area to match the area currently displayed in the contour map, *right-click* the video image and choose Match Chemical Image Size from the pop-up menu.

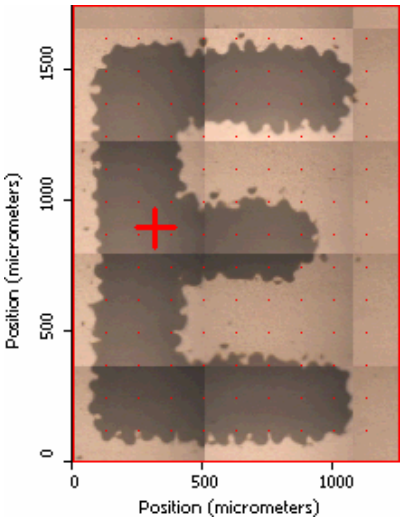
Examples of a video image for a line map, area map and discrete point map are shown below. The video image for a line depth profile would be similar to that for a line map, except that no line would appear. The video image for an area depth profile would be similar to that for an area map, except that a line would appear instead of sample points.

For a line map the location of the line formed by the sample points is indicated in the video image by a red line. The cross hairs (or other cursor type) show the location of the sample point that corresponds to the currently displayed spectrum.



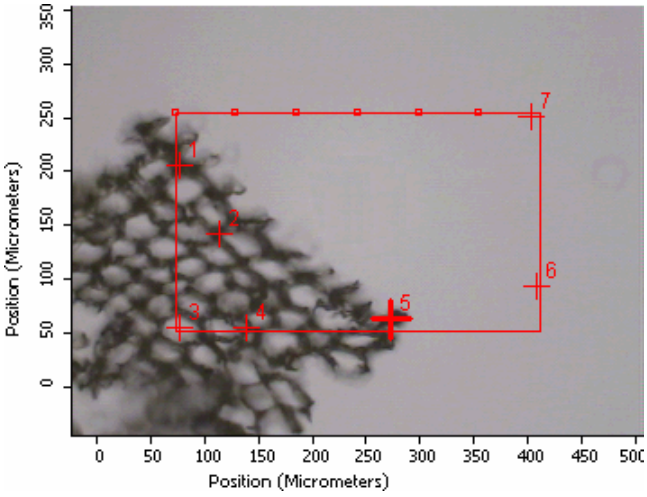
Line map video image

The locations of the sample points are indicated in the video image by red dots. The cross hairs (or other cursor type) show the location of the sample point that corresponds to the currently displayed spectrum.



Area map video image

The locations of the sample points are indicated in the video image by numbered cross hairs.



Discrete point map video image

If you move the cross hairs (or other cursor type) in the video image for a line map or area map, the spectrum collected at the new location appears in the spectral display pane (if present). To do this, click a location in the video image, drag the cross hairs (or other cursor type), or use the arrow keys on the keyboard when the video pane is active.

Note If a line icon or "T" appears next to the pointer, do the following before clicking a point or dragging the cross hairs: *Right-click* the contour map (or discrete point location map), point to Cursor Mode and choose Select And Zoom from the pop-up menu. ▲

If you added markers when you set up the map collection, you can display them in the video image by *right-clicking* the image and choosing Show Markers from the pop-up menu. A check mark appears next to the command name when the markers are displayed. To remove the markers from the video image, *right-click* the image and choose Show Markers again. You can also toggle the display of markers by using Show Map Markers on the Video tab of the Display Setup dialog box. See "Displaying markers" for more information. See "Adding a marker" in the "Preparing for Data Collection" chapter for information about adding markers.

You can measure items in the video image: *Right-click* the image, point to Cursor Mode, choose Ruler from the pop-up menu, and then drag across the image to draw a ruler. (The ruler also appears on the contour map.) The measured distance appears near the bottom of the map window. You can manipulate the ruler just as you would in the Atlμs window. See "Moving the ruler" and "Resizing the ruler" in the "Preparing for Data Collection" chapter if you need help. To remove the ruler, *right-click* the image, point to Cursor Mode and choose Select And Zoom from the pop-up menu.

You can add annotation to the video image:

1. *Right-click* the image, point to Cursor Mode and choose Annotation from the pop-up menu.

2. Click the desired location in the video image.

3. Type the desired text in the box that appears.

4. Click outside the box.

To specify whether this annotation is displayed, use Show Video Annotation on the Video tab of the Display Setup dialog box. (See "Setting the video annotation parameters" for details.) To delete the added annotation, click it while the cursor is in Annotation mode, delete the text using the keyboard, and then click outside the box.

Use the Video tab of the Display Setup dialog box to change how the video image is displayed. See "Video display parameters" for details.

You can overlay the video image with the contour map (or discrete point location map) to see spatial relationships between the two. (This feature is not available for depth profiles.) See "Overlaying the video image and contour map or discrete point location map" for details.

You can save the video image as a .bmp, .jpg or .tif file by *right-clicking* the image and choosing Save from the pop-up menu. Specify a file name and location in the dialog box that appears and then choose Save. You can open the file later using a program that opens files of its type. You can also save the video image by using Save Video Image in the File menu. See "Saving the video image" in the "Preparing for Data Collection" chapter for details.

Spectral display pane

If Spectrum is selected on the Mapping - General tab of the Display Setup dialog box, a spectral display pane appears in the map window or profile window. It shows the spectrum collected at the location indicated by the cross hairs (or other cursor type) on the video image. (In the case of a depth profile, the pane shows the spectrum collected at the location indicated on the contour map.) This spectrum also corresponds to the indicated location on the 3-D image and contour map (or discrete point location map).

For a line map, area map or discrete point map, you can display a different spectrum by clicking the desired location in the video image, 3-D image or contour map (or discrete point location map).

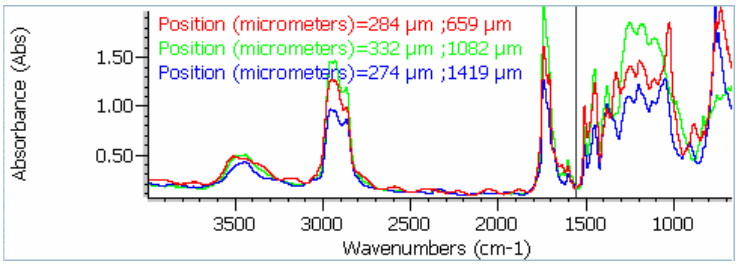
For a depth profile, you can display a different spectrum by clicking the desired location in the 3-D image or contour map.

You can display multiple spectra by holding down the Shift key while you click locations. If the contour map (or discrete point location map) or video pane is active, you can drag the cross hairs (or other cursor type) to a different location or use the arrow keys on the keyboard.

The vertical line in the pane corresponds to the middle vertical line in the view finder and works in a similar manner. By dragging it, you can specify a frequency to use for displaying data in some of the panes. See the description of the view finder in "Using map windows" for more information.

The pane may include axis labels depending on the settings of X-Axis Label and Y-Axis Label on the Mapping - General tab. See "Setting the spectral display parameters" for more information.

In the upper-left corner of the pane are the titles of the displayed spectra. Here is an example:



You can remove the spectral display pane from the window by *right-clicking* it and then choosing Hide from the pop-up menu.

Using the 3-D display

If you have selected 3-D Image on the Mapping - General tab of the Display Setup dialog box, the map window or profile window contains a 3-D image.

You can rotate the 3-D image in any direction to see the data from different angles. Simply drag the image in the direction you want to rotate it; the image rotates as you move the mouse. Release the mouse button when you have displayed the desired view of the data. If you release the mouse button while the mouse is moving (and the image is still rotating), the image will continue to rotate. This can help you study the shape of the data from all sides.

Use the 3-D View tab of the Display Setup dialog box to change how the 3-D image is displayed. See "3-D View display parameters" for details.

Note You can remove the 3-D display from the window by *right-clicking* it and then choosing Hide from the pop-up menu. ▲

The next sections describe the 3-D image displayed for line maps, area maps and depth profiles.

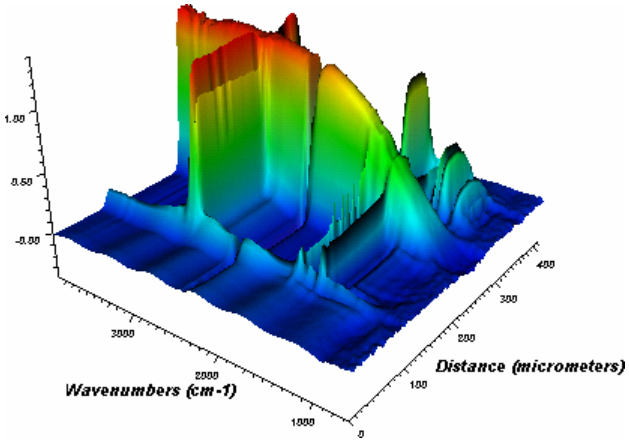
3-D image for line maps and line depth profiles

For a *line map*, the 3-D display shows an image of the map data in these three dimensions: distance in micrometers from the first sample point (Distance axis), frequency (Wavenumbers axis) and spectral intensity (vertical axis).

For a *line depth profile*, the 3-D display shows an image of the map data in these three dimensions: distance in micrometers from the zero point (Depth axis), frequency (Wavenumbers axis) and spectral intensity (vertical axis).

The use of color in the 3-D image is specified by the color bar (see "Using map windows" for more information). The image shows data from the portion of the map specified by the sky view control.

The following illustration shows an example of a line map 3-D image in the form of a surface plot (a warped, interpolated surface) showing spectral intensities at different frequency (wavenumber) and distance locations. A 3-D image for a line depth profile would be similar, except that the Distance axis would be labeled "Depth."



Line map 3-D image displayed as a surface plot

See "3-D View display parameters" for more information about displaying the 3-D image for line maps.

3-D image for area maps and area depth profiles

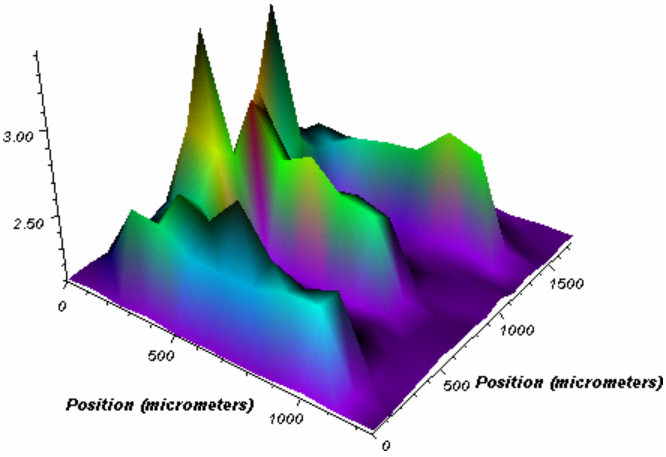
There are two fundamental ways to display a 3-D image for an area map or area depth profile:

For an *area map you* can display a surface plot (select Show Surface in the Display Setup dialog box) with these three dimensions: X position and Y position on the microscope stage (the two Position axes) and value (vertical axis). The image is essentially a conversion of the contour map to a three-dimensional form that makes it easier to see the values across the sample.

For an *area depth profile* you can display a surface plot (select Show Surface in the Display Setup dialog box) with these three dimensions: distance along the top edge of the mapped vertical area (the Position axis), Z position relative to the zero point (the Depth axes) and value (vertical axis). The image is essentially a conversion of the contour map to a three-dimensional form that makes it easier to see the values across the vertical area of the depth profile.

In addition to representing values by colors, the 3-D image uses surfaces within which intensity peaks can be located.

Here is an example of an area map 3-D image in the form of a surface plot (a warped, interpolated surface) showing values at different locations on the sample:



Area map 3-D image displayed as a surface plot

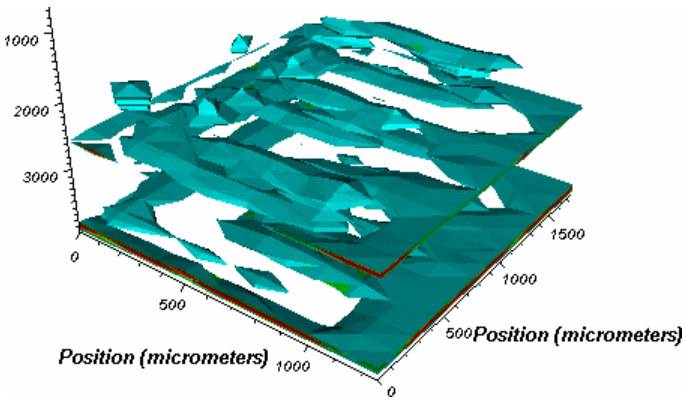
This type of 3-D image represents a part (or "slice") of the volume of the area map data, with one dimension (frequency) held constant. In the example above, the image shows spectral intensities at a single frequency (specified by the vertical line in the spectral display pane and view finder).

By selecting Show Full Volume in the Display Setup dialog box, you can also display the full volume of the area map or area depth profile:

For an area map this display has these dimensions: X position and Y position on the microscope stage (the two Position axes) and spectral frequency (vertical axis).

For an area depth profile this display has these dimensions: X position and Z position (the two Position axes) and spectral frequency (vertical axis).

The surfaces displayed in the same color represent areas of similar intensity. The values indicated by the colors are specified by the color bar. Here is an example of a 3-D image showing full volume:



Full volume displayed in 3-D image

In both surface-plot and full-volume 3-D images, the image shows data from the portion of the map specified by the sky view control.

See "3-D View display parameters" for more information about displaying the 3-D image for area maps.

Profile panes

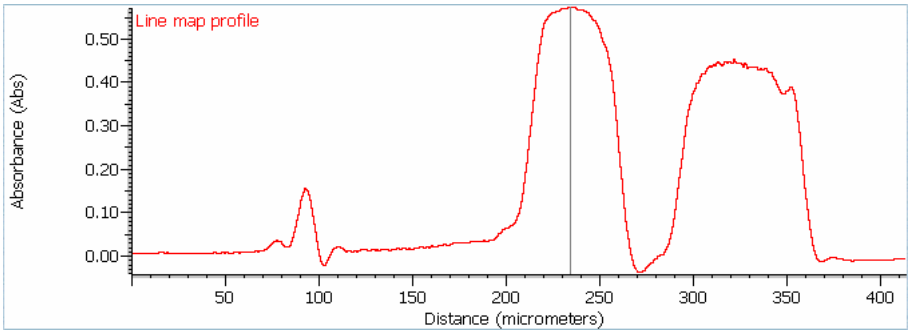
If Profile is selected on the Mapping - General tab of the Display Setup dialog box, the map window or profile window contains one or more profile panes. The next sections describe how these panes are used for line maps (and line depth profiles) and area maps (and area depth profiles).

You can copy a profile pane to the Windows Clipboard by *right-clicking* the pane and choosing Copy from the pop-up menu. You can then paste the image into a spectral window, or into a document using a program that pastes items from the Clipboard.

If you have zoomed in on a spatial area using the contour map, video image or sky view control, you can redisplay the entire spatial range by *right-clicking* a profile pane and choosing Full Range from the pop-up menu.

Profile pane for line maps and line depth profiles

If you are displaying a line map or line depth profile, the single profile pane of the map window or profile window shows spectral intensity at the current frequency (specified by the middle vertical line in the view finder) versus distance along the line map or line depth profile. Here is an example:



Line map profile pane

The X location of the vertical gray line in the profile pane corresponds to the location of the current spectrum on the line map or line depth profile.

For a line map this location is indicated by the cross hairs (or other cursor type) in the video image (or on the contour map or 3-D image). When you click a different location, the line in the profile pane moves accordingly.

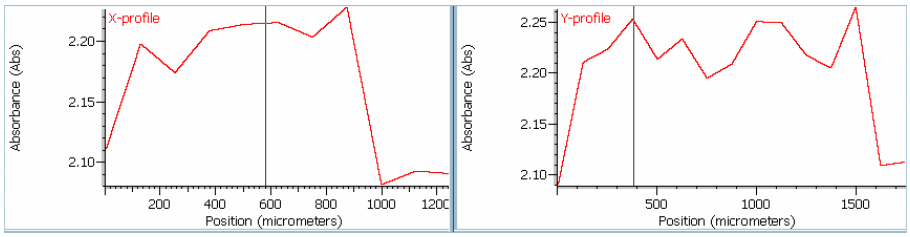
For a line depth profile the spectrum location is indicated by the cursor on the contour map (or 3-D image). When you click a different location, the line in the profile pane moves accordingly.

You can drag the line in the profile pane to a new location. The other panes are updated accordingly.

Profile panes for area maps and area depth profiles

If you are displaying an area map or area depth profile, two profile panes are needed.

For an *area map*, the X-direction profile shows the spectral intensity at the current frequency (specified by the middle vertical line in the view finder) of the spectra collected at sample points having the same Y coordinate value versus the X coordinate value. Similarly, the Y-direction profile shows the spectral intensity at the current frequency of the spectra collected at sample points having the same X coordinate value versus the Y coordinate value. Here is an example:



Area map profile panes

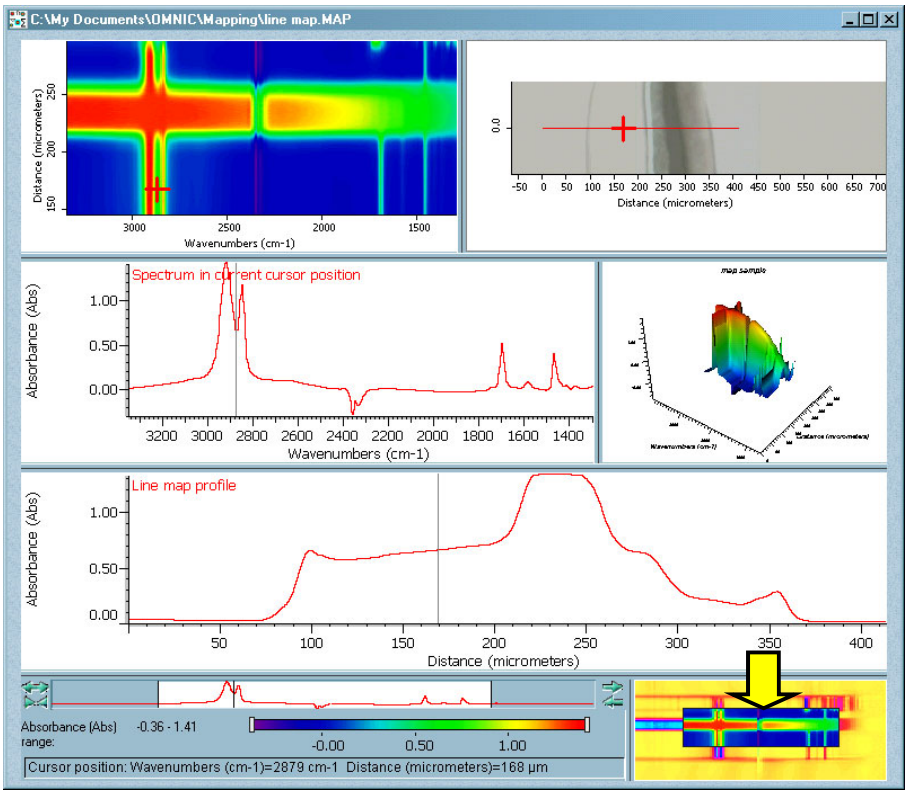
The vertical gray lines in the profile panes correspond to the X and Y locations of the current spectrum, whose location is indicated by the cross hairs (or other cursor type) in the video image. The locations of the lines move when you click a different location in the video image.

Adjusting the display with the sky view control

The sky view control lets you quickly change the display of map data. It is filled with an image of the entire contour map (or discrete point location map). Within the control is a box that indicates the portion of the map data currently visible in some of the other parts of the window. (When you first open a map, this box is the same size as the control itself.) The portion of the sky view control outside the box is displayed in reverse video colors.

Here is an example showing how the box in the sky view control indicates the displayed portion of a *line map* (or line depth profile):

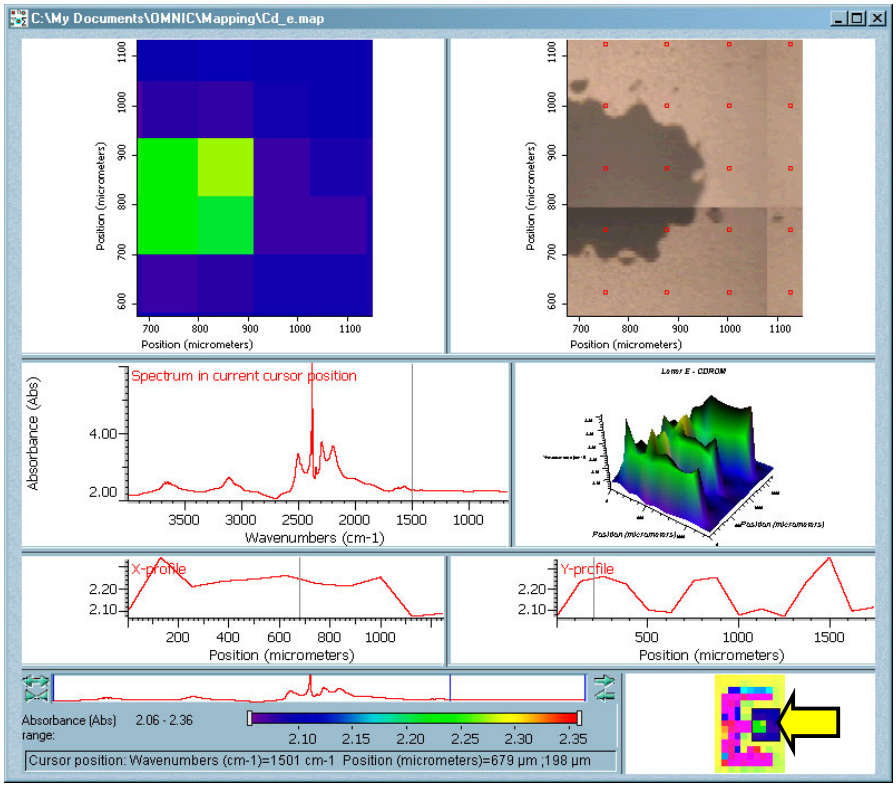
Notice that the box in the sky view control (at the end of the arrow) corresponds to the data shown in the contour map, spectral display pane, 3-D image and view finder.



Line map zoomed in with sky view control

Here is an example showing how the box in the sky view control indicates the displayed portion of an *area map* (or area depth profile):

Notice that the box in the sky view control (at the end of the arrow) corresponds to the data shown in the contour map and the portion of the sample visible in the video image.



Area map zoomed in with sky view control

Use the instructions that follow to adjust the display using the sky view control.

Changing a display limit – Drag any side of the box to change the display limit that corresponds to that side.

Displaying a different area of the same size – There are two ways to do this. You can simply drag the box to the desired location. As you drag the box, an outline remains in the original location until you release the mouse button.

You can also click a point outside the box. The new display area is centered (if possible) at the point you clicked.

Changing the size and shape of the displayed area – Drag any corner of the box to change either the box's size or shape or both.

Displaying the entire map – To display the entire map, double-click inside the box.

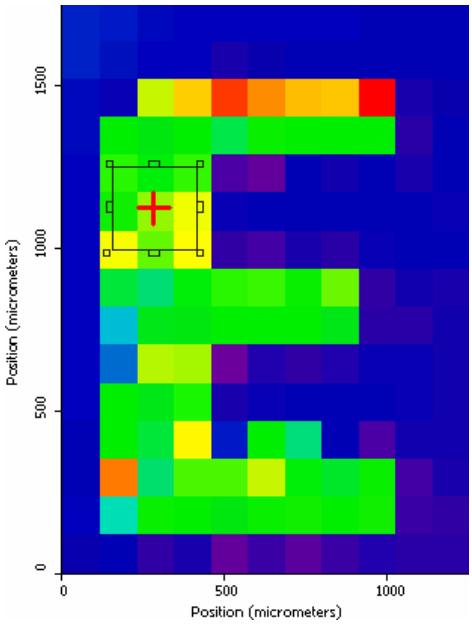
Zooming in and out on map data

Follow these steps to zoom in on your map data:

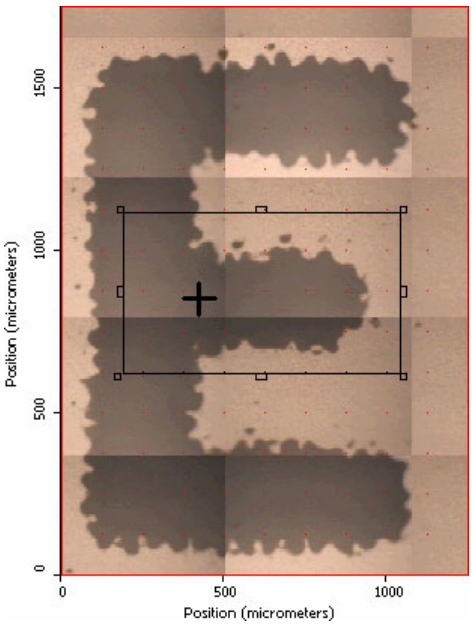
1. **Use the mouse to draw a box around the area of interest in the contour map (or discrete point location map).**

Note If a line icon or "T" appears next to the pointer, first *right-click* the contour map (or discrete point location map), point to Cursor Mode and choose Select And Zoom from the pop-up menu. ▲

Here is an example:



If you are displaying an area map or discrete point map, you can also draw a box in the video image. Here is an example showing a box drawn around a different area:



2. **If desired, drag the handles on the sides or corners of the box to adjust its size and shape.**

3. **Click inside the box.**

   The area expands and the 3-D image and spectral display pane change to reflect the new display limits.

   To redisplay the full data range, *right-click* the 3-D image, video image, spectral display pane, profile pane or contour map (or discrete point location map) and then choose Full Range from the pop-up menu. If the video pane contains a Mosaic, the entire Mosaic is displayed when you choose Full Range.

Note You can also use the spectral display pane, sky view control or view finder to expand an area of map data. For details see "Zooming in on an area in the spectral display pane" or "Adjusting the display with the sky view control" in this chapter or "View finder" in the OMNIC Help system (find "view finder" in the Help system Index). ▲

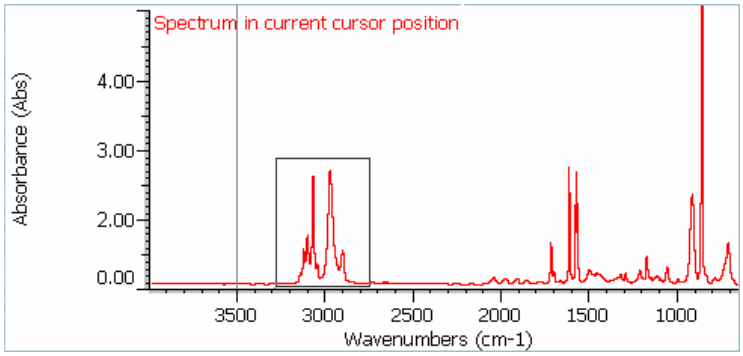
Zooming in on an area in the spectral display pane

Follow these steps to zoom in on an area in the spectral display pane:

1. **Use the mouse to draw a box around the area of interest in the spectral display pane.**

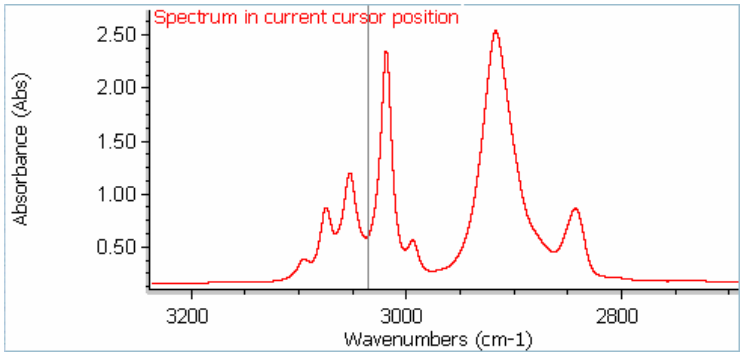
   If the cursor is in region mode (two vertical lines with triangular handles appear in the pane), first *right-click* anywhere in the pane, point to Cursor Mode in the pop-up menu and then choose Zoom. You can then draw a box in the pane.

   Here is an example:



2. **Click inside the box.**

   The boxed area expands to fill the pane:



- If you are displaying a line map or line depth profile, the contour map, 3-D image, view finder and sky view control also change to reflect the new frequency limits. The vertical gray line in the spectral display pane moves if necessary to be visible within the displayed spectral region. If it moves, the profile pane changes to reflect the new frequency location of the line.

- If you are displaying an area map or area depth profile, the 3-D display also changes to reflect the new frequency limits. The vertical gray line in the spectral display pane moves if necessary to be visible within the displayed spectral region. If it moves, the contour map, sky view control and profile panes change to reflect the new frequency location of the line.

- If you are displaying a discrete point map, the view finder also changes to reflect the new frequency limits. The vertical gray line in the spectral display pane moves if necessary to be visible within the displayed spectral region.

To redisplay the full data range, *right-click* the 3-D image, video image, spectral display pane, profile pane or contour map (or discrete point location map) and then choose Full Range from the pop-up menu. If the video pane contains a Mosaic, the entire Mosaic is displayed when you choose Full Range.

Animating your view of the map data

Choose Animation from the Atlμs menu to see an animated display of the changes that occur in your area map data as the spectral frequency changes. The command automatically moves the middle vertical line in the view finder to the right, stepping through the displayed frequency range of the data. The contour map, 3-D image and profiles (if displayed) change to reflect the new frequency.

To change the speed of movement, drag the vertical bar left or right along the Animation Speed control below the view finder.

To stop the animation, press the Esc key on the keyboard, click anywhere within the view finder, or choose Animation again. This removes the check mark from in front of the command name.

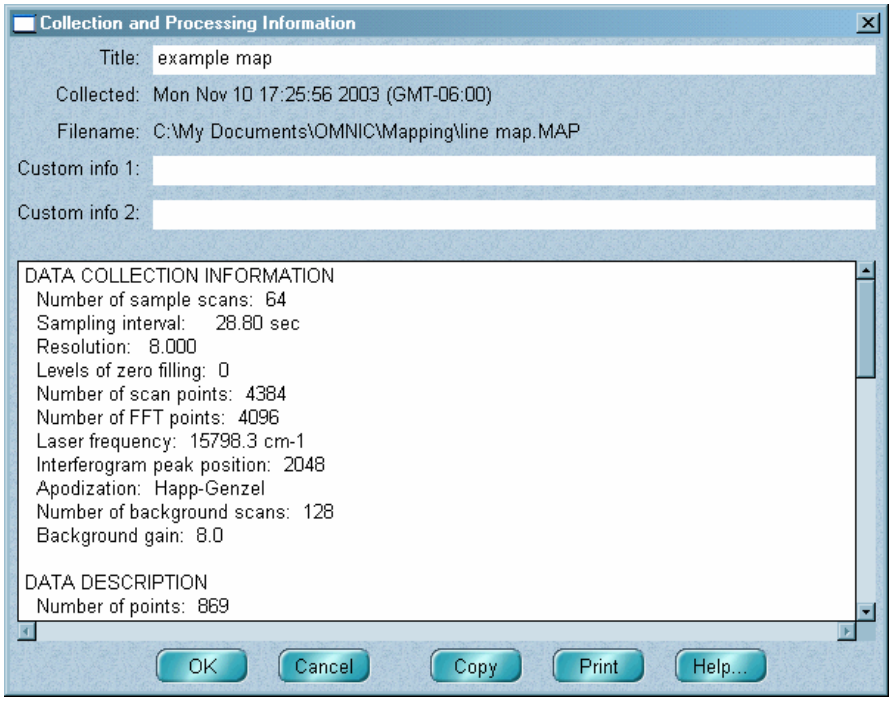
Copying the 3-D image, video image, displayed spectra or contour map

You can copy to the Windows Clipboard the 3-D image, the video image, the last spectrum to be displayed in the spectral display pane or all the spectra in the pane, or the contour map (or discrete point location map). Simply *right-click* the item you want to copy and choose Copy from the pop-up menu. To copy all the spectra in the spectral display pane, first choose Select All from the Edit menu. You can then paste the copied item into programs that allow pasting from the Clipboard. If you copy spectra, you can paste them into a spectral window.

Viewing information about a map

If a map window is active, you can use Show Map Info in the Atlμs menu to view information about the map, including how it was collected. You can also change the title of the map, enter comments about the map or copy or print the map information.

The information is displayed in the Collection And Processing Information window. Here is an example showing the special mapping information scrolled into view:



This is essentially the same window that appears when you click the Information button ("i") in a spectral window or double-click a spectrum title in the title box.

For more information about this window, choose OMNIC Help Topics from the Help menu, find "collection and processing information" in the Index and go to the "Collection and processing information" topic.

Follow these steps to view information about a map:

1. **Choose Show Map Info from the Atlμs menu.**

   The Collection And Processing Information window appears.

2. **To change the map title, edit the title directly in the Title text box.**

3. **To see information about the map, use the scroll bars to scroll the desired information into view.**

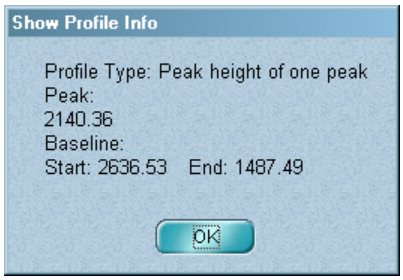
   You can copy all the information in the window to the Windows Clipboard by choosing Copy. You can then paste the information using another Windows application that uses the Clipboard.

   You can print all the information on the default system printer by choosing Print.

4. **When you are finished viewing the information, choose OK to close the window and save any changes you made, or choose Cancel to close the window without saving your changes.**

Viewing information about a profile

Choose Show Profile Info from the Atlμs menu to view information about the profile in the active profile window. Here is an example:



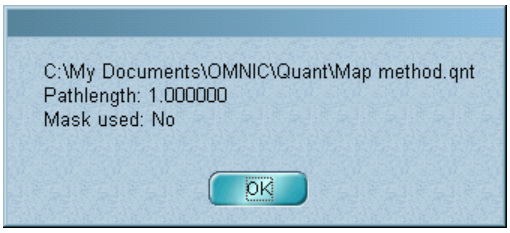
To close the dialog box, choose OK.

For information about creating a profile, see “Creating a profile” in the “Processing and Analyzing Map Data” chapter.

For information about displaying the current profile for an area map, see “Displaying the current profile or a saved profile” in the “Displaying Map Data” chapter.

Viewing information about quantitative analysis results

If the active window displays the results of quantifying a map, you can choose Show Quant Info from the Atlμs menu to view information about the results. Here is an example:



To close the dialog box, choose OK.

For information about quantifying a map, see “Quantifying a map” in the “Processing and Analyzing Map Data” chapter.

Setting the display parameters

Use Display Setup in the View menu to specify how to display data in the active map window, profile window or PCA result window. Other windows on the screen are not affected.

Note If you choose Display Setup when a spectral window is active, the dialog box contains only parameters that are appropriate for a spectral window. In OMNIC Help Topics find "display parameters" in the Index and go to "Setting the display parameters" for information about setting those parameters. ▲

You can set some of the display parameters before map collection. See "Setting the mapping options" in the "Preparing for Data Collection" chapter for more information.

Follow the steps below to set the display parameters for the active map window or profile window. The next sections describe the parameters in detail.

1. **Choose Display Setup from the View menu.**

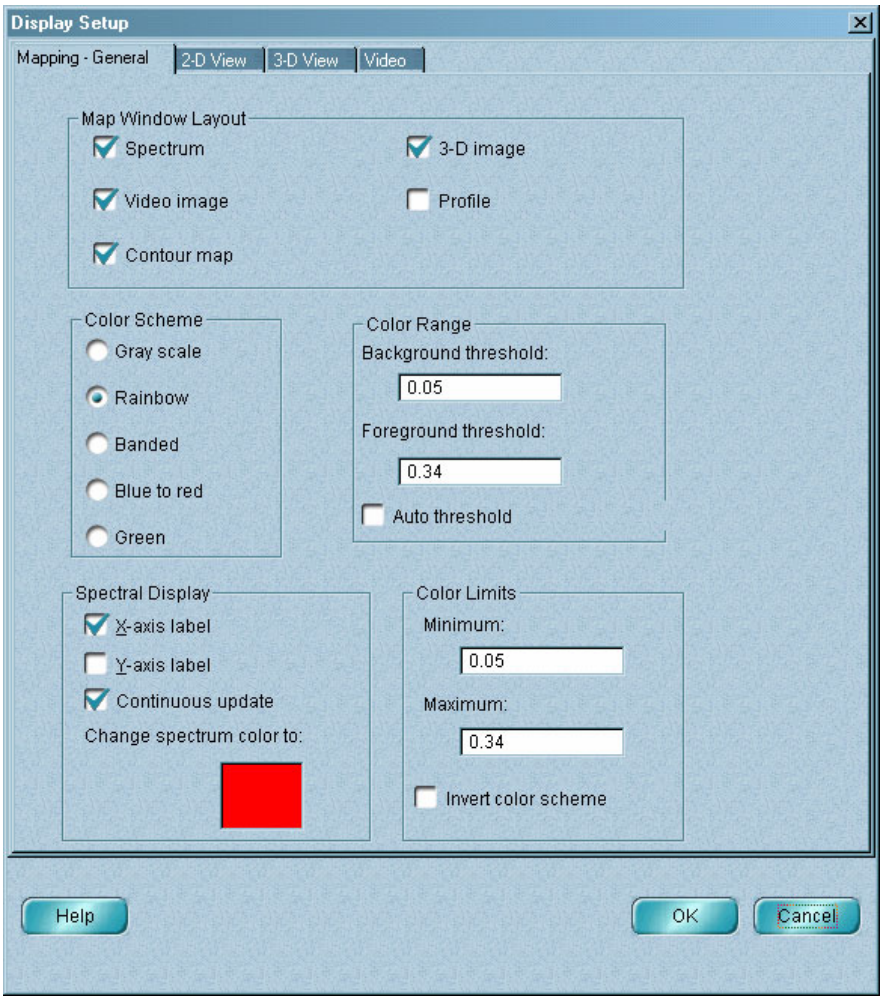
   The Display Setup dialog box appears. See the next section for an illustration.

2. **Set the display parameters.**

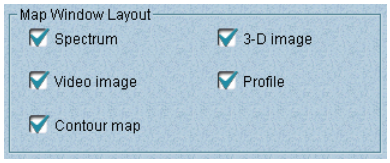
3. **Choose OK.**

Mapping – General display parameters

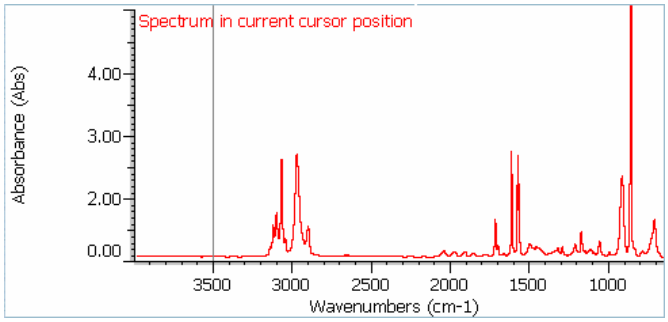
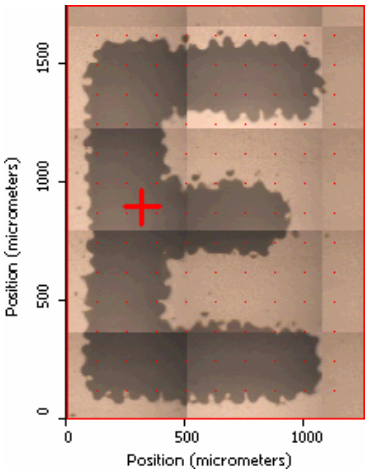
This section explains the display parameters available on the Mapping - General tab:

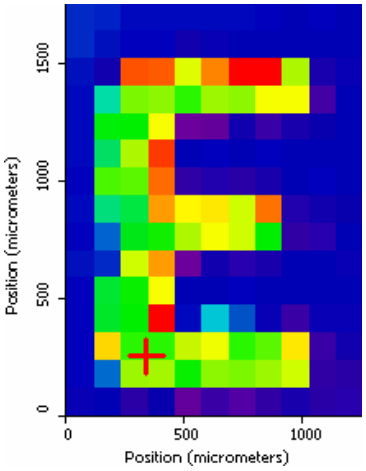
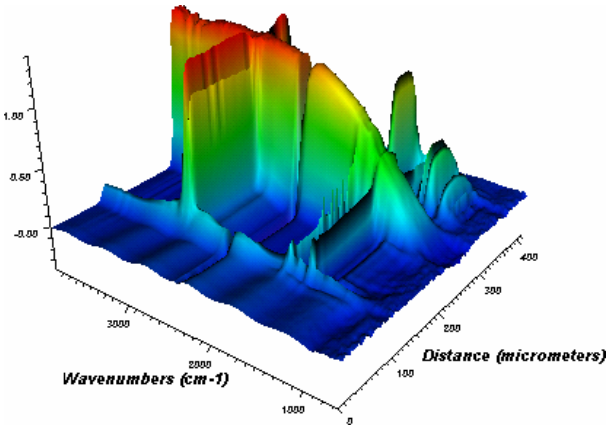


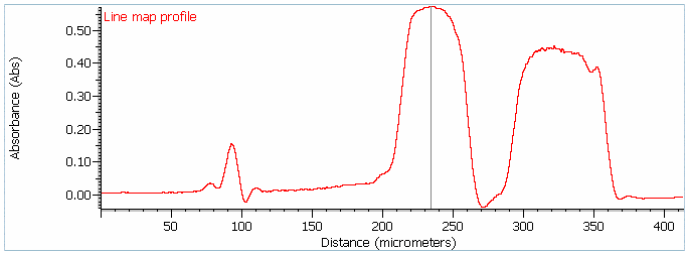
Specifying the items to display



Select the items in the Map Window Layout box that you want displayed in the active map window or profile window. The table below describes the available items and shows examples. Each item is displayed in its own pane, whose size and shape you can adjust (see "Using map windows").

Select this…	To display this…
Spectrum	Spectral display pane containing the map spectrum that corresponds to the specified location in the video image or contour map (or discrete point location map). 
Video Image	Video image or Mosaic of the sample. This item is available only if a video image or Mosaic was captured and saved with the map. 

Select this…	To display this…
Contour Map	Line contour map, area contour map, depth profile contour map, or discrete point location map. 
3-D Image	3-D image of map data. This item is not available for discrete point maps, since they are collected at individually specified sample points that may not be uniformly spaced. 

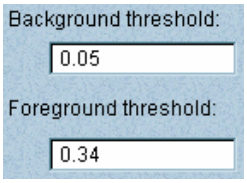
Select this…	To display this…
Profile	Profile or profiles of the map data. This item in not available for discrete point maps. 

Selecting a color scheme

Specify a color scheme for your contour map (or discrete point location map) and 3-D image by selecting an option in the Color Scheme box. The table below describes how each option represents values.

Color Scheme	Description
Gray Scale	Uses shades of gray along a gradient to represent values. This option is useful for printing contour maps (or discrete point location maps) and 3-D images on a black-and-white or gray-scale printer. Since the values change as the gray shades become darker, it is easy to identify areas of relative low and high value on the printed map or image. If you print a colored contour map (or discrete point location map) or 3-D image on the same printer, however, the darkness of the resulting printed gray shades will not necessarily correlate with the values. A color that represents a high value, for example, may appear as a light gray on paper. This option is also useful for seeing contrast in the display of data.
Rainbow	Uses a gradient of blended rainbow colors to represent values.
Banded	Uses bands of colors, rather than a gradient of blended colors, to represent values.
Blue To Red	Uses blended colors from blue to red to represent values.
Green	Uses blended shades of green to represent values.

Specifying the background and foreground thresholds



Background Threshold and Foreground Threshold let you specify the limits of the value range used for the colors in the contour map and 3-D image. Type the desired limits in the text boxes. The limits must be within the range specified in the Color Limits box. See "Setting the color limits" for details.

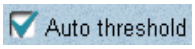
For a line map, line depth profile or discrete point map the Background Threshold value represents the minimum spectral intensity, and the Foreground Threshold value represents the maximum spectral intensity.

For an area map or area depth profile the Background Threshold value represents the minimum value of the specified type, and the Foreground Threshold value represents the maximum value of the specified type.

You can also set the range by dragging the vertical bars on the color bar. See "Using map windows" for more information.

See the next section for setting the thresholds automatically.

Setting the thresholds automatically

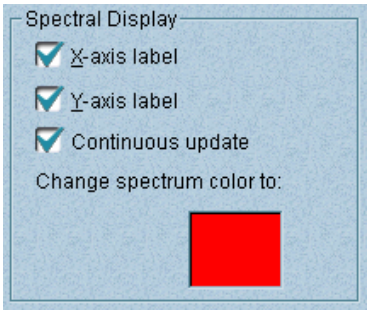


Select Auto Threshold if you want the background and foreground thresholds automatically adjusted to provide the most variation whenever you perform any of the following operations:

- Process a map using a command in the Process menu.
- Truncate the spectral range of a map using Truncate Data Set in the Atlμs menu.
- Create an area map profile using Profile Setup in the Atlμs menu.

Note You can also select this option by *right-clicking* the contour map and then choosing Auto Threshold from the pop-up menu. ▲

Setting the spectral display parameters

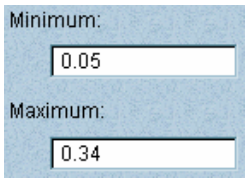


Select X-Axis Label and Y-Axis Label if you want the X-axis and Y-axis of the spectral display pane to be labeled with their units.

Select Continuous Update if you want the data in the affected panes to be updated while you move the middle vertical line in the view finder or the vertical line in the spectral display pane. (See the description of the view finder in "Using map windows" for more information.) If this option is not selected, the affected panes are updated when you release the mouse button after dragging the line.

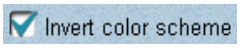
The color in the box to the right of Change Spectrum Color To shows the color used for displaying the selected spectrum in the spectral display pane. To change the color, click the box. The Color dialog box (a Windows feature) appears allowing you to select a color. If you need help using the features in this dialog box, click the "?" button and then click the feature of interest. When you are finished selecting a color, choose OK.

Setting the color limits



Use Minimum and Maximum in the Color Limits box to specify the range of available values for the color bar. Type the desired minimum and maximum values in the appropriate text boxes. See "Using map windows" for information about how the color bar uses this range. See "Specifying the background and foreground thresholds" for information about setting the limits of the value range used for the colors in the contour map and 3-D image.

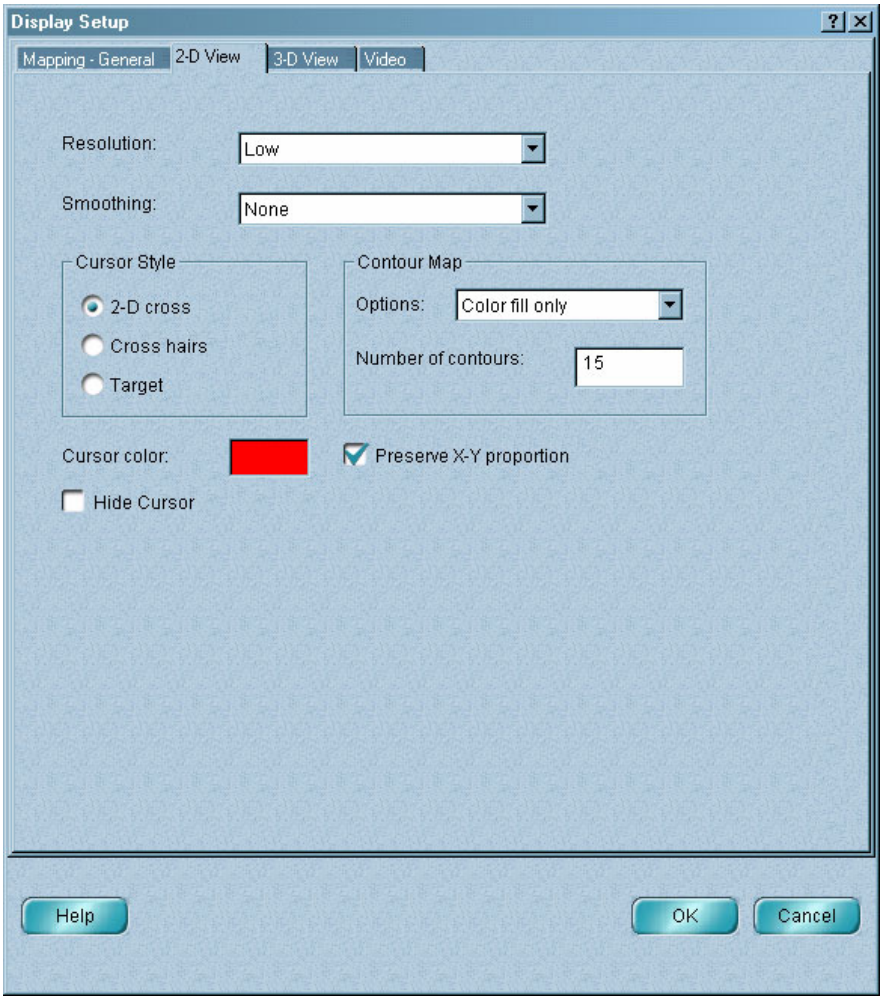
Inverting the color scheme



You can reverse the order of the colors in a color scheme by selecting Invert Color Scheme.

2-D View display parameters

This section explains the display parameters available on the 2-D View tab:

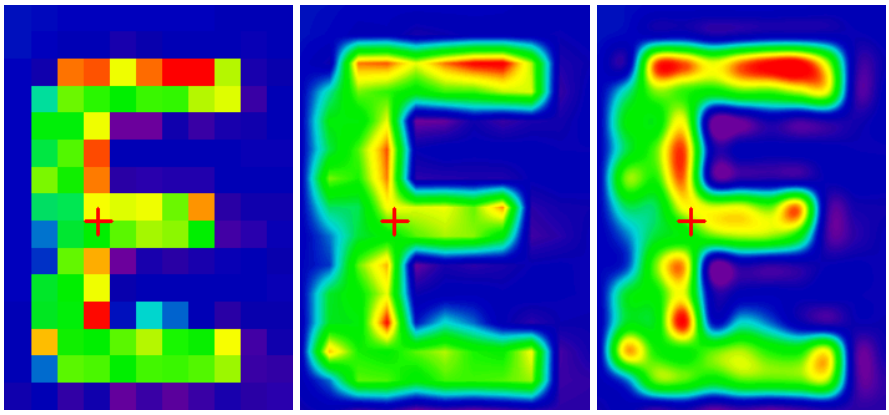


Selecting the resolution for the contour map

If you are using linear or spline smoothing (see the next section), specify the resolution for the contour map by setting Resolution. Increasing the resolution increases the degree of detail and smoothness of the map, but the software may respond more slowly when you change the display of data. (If you are displaying a discrete point location map, this parameter has no effect.)

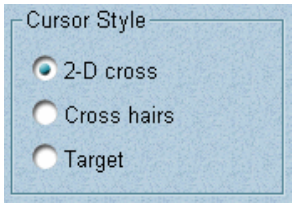
Selecting the smoothing type for the contour map

Specify the type of smoothing to use for the contour map by setting Smoothing. The Spline setting results in greater smoothing than the Linear setting. Select None if you don't want to smooth the map. See the examples below. (If you are displaying a discrete point location map, this parameter has no effect.)

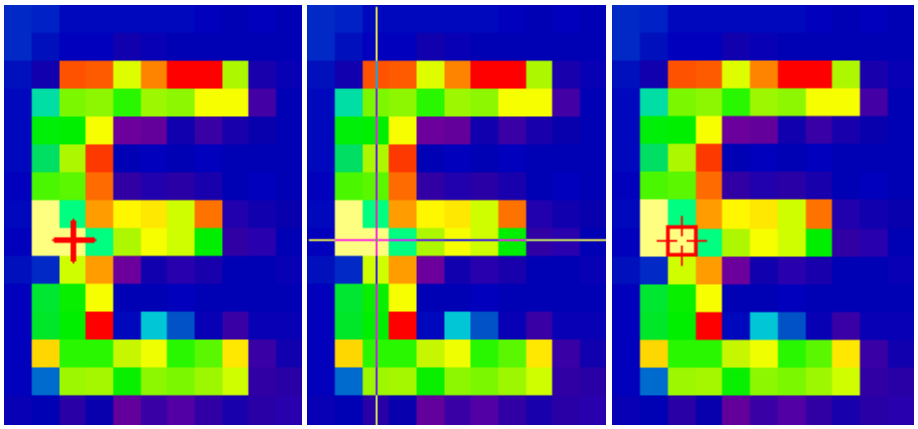


None Linear Spline

Selecting a cursor style for the contour map or discrete point location map

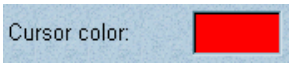


Specify a cursor style for the contour map (or discrete point location map) by selecting an option in the Cursor Style box. The available styles are shown below.



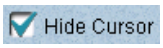
2-D Cross Cross Hairs Target

Specifying a color for the contour map or discrete point location map cursor



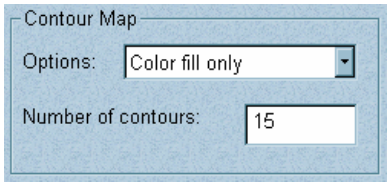
The color in the box to the right of Cursor Color shows the color used to display the contour map (or discrete point location map) cursor. To change the color, click the box. The Color dialog box (a Windows feature) appears letting you select a color. If you need help using this dialog box, click the "?" button and then click the feature of interest. When you are finished selecting a color, choose OK.

Hiding the contour map or discrete point location map cursor

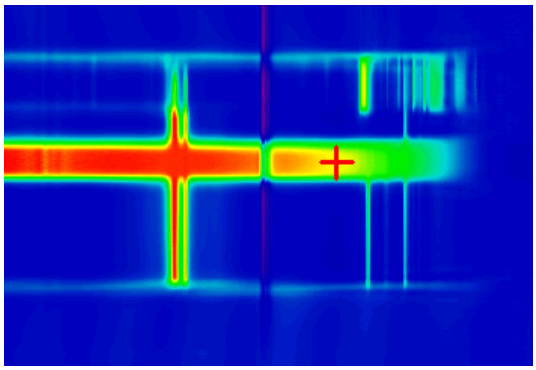


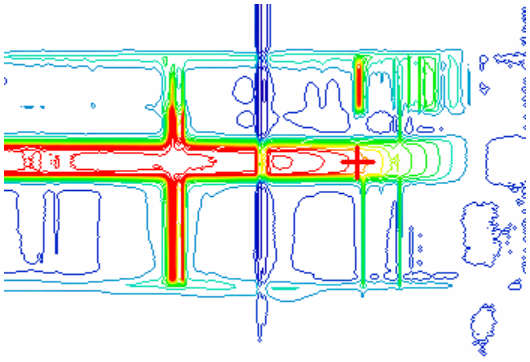
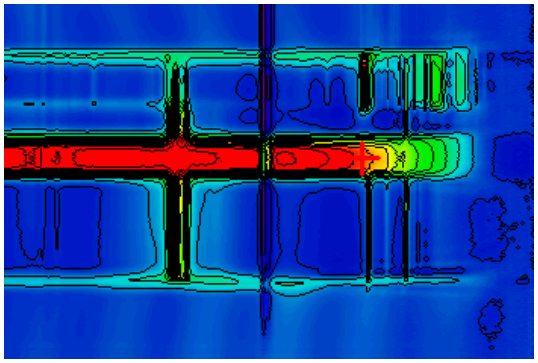
If you want to hide the cursor for the contour map (or discrete point location map), select Hide Cursor.

Setting the contour parameters



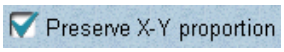
The features in the Contour Map box let you specify how to display the contour map. The table below describes the available settings of Options and shows examples of the map elements they display. (The settings do not affect points in a discrete point map, which are always displayed in solid colors representing spectral intensities.)

Select this…	To display this…
Color Fill Only	Areas of solid color without lines separating the areas.  For a line map or line depth profile the areas represent ranges of spectral intensity. For an area map or area depth profile the areas represent the specified type of value.

Select this…	To display this…
Contour Lines Only	Colored contour lines (“isolines”) with the areas between the lines not filled with color.  For a line map or line depth profile the lines represent single spectral intensities. For an area map or area depth profile the lines represent the specified type of value.
Contour Lines And Color Fill	Areas of solid color with black lines separating the areas.  For a line map or line depth profile the areas represent ranges of spectral intensity. For an area map or area depth profile the areas represent the specified type of value.

Type the desired number of contours in the Number Of Contours text box. Increasing the number of contours makes the change in contour value from one location to another appear more gradual and smoothes the edges of shapes in the map.

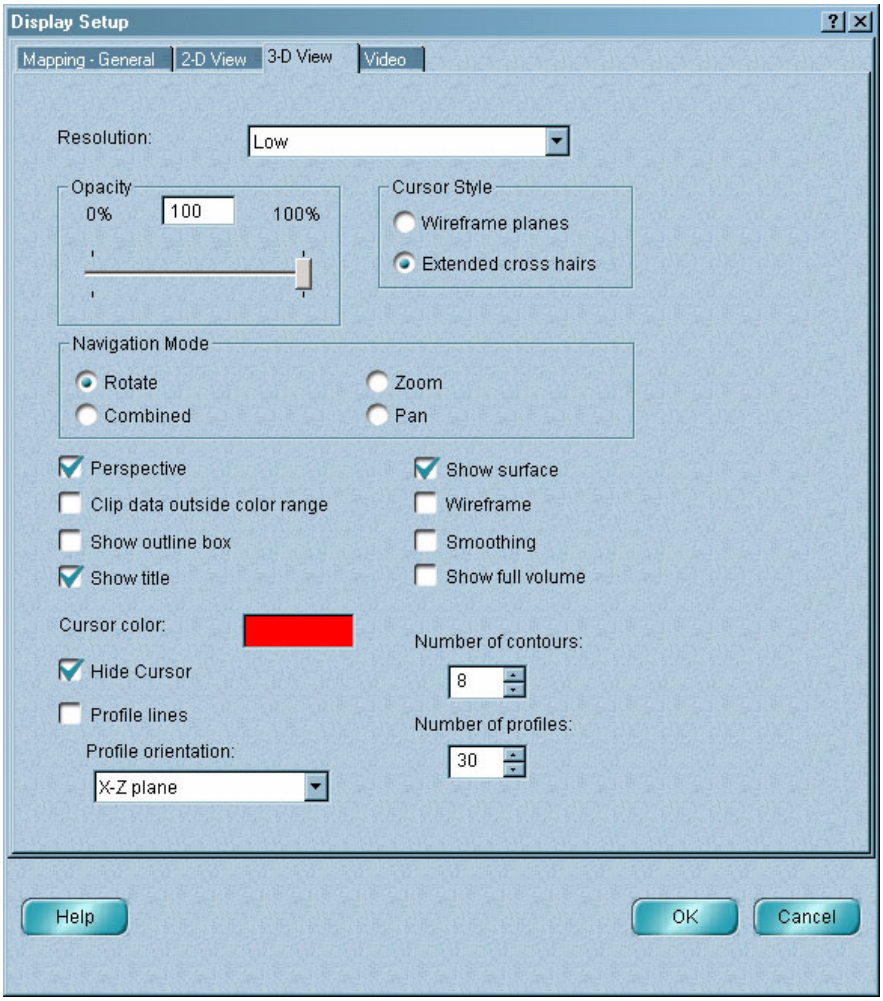
Preserving the X-Y proportion



Select Preserve X-Y Proportion if you want the shape of the contour map (or discrete point location map) maintained when you resize the map (by dragging the borders of its pane or by resizing the map window or profile window). If this option is not selected, the height and width of the map can change independently when you resize the map.

3-D View display parameters

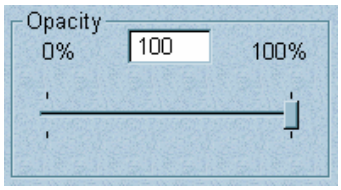
This section explains the display parameters available on the 3-D View tab:



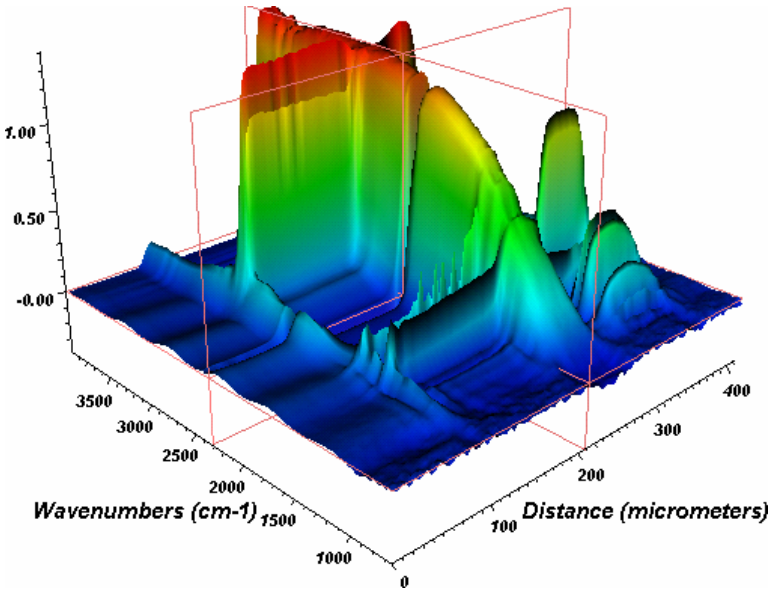
Selecting the resolution of the 3-D image

Specify the relative resolution of the 3-D image by setting Resolution. Increasing the resolution increases the degree of detail and smoothness of the image. However, this can slow the rendering of the image and your interactions with it (such as zooming in and rotating the image).

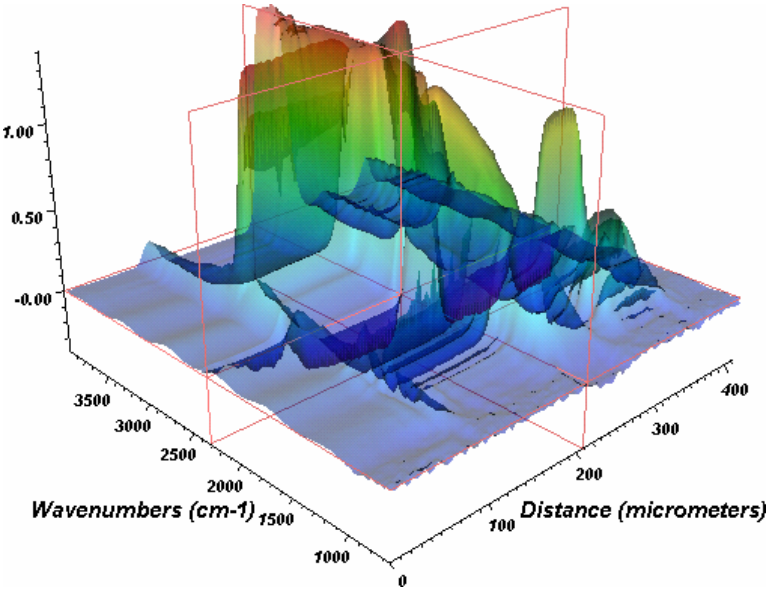
Setting the opacity of the 3-D image



Set the opacity of the 3-D image by typing a number from 0 to 100 in the text box in the Opacity box or by dragging the small vertical bar below the text box to the left or right. Reducing the opacity lets you see peak shapes through other, closer peaks as though they were translucent. The illustrations below show the effects of changing the opacity from 100% to 50%.

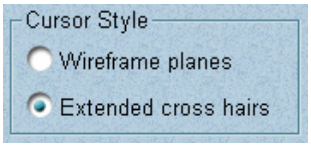


100% opacity

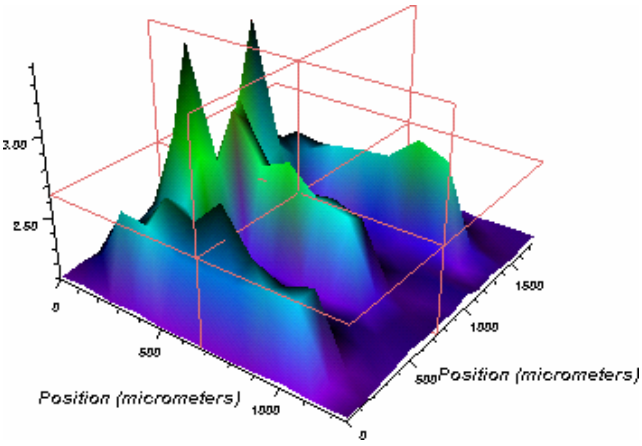


50% opacity

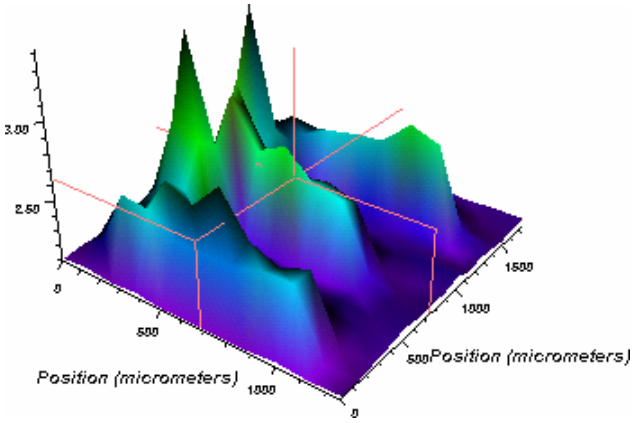
Selecting a cursor style for the 3-D image



Specify a cursor style for the 3-D image by selecting an option in the Cursor Style box. The Wireframe Planes option displays outlines of three imaginary orthogonal (perpendicular) planes that intersect at the cursor location. Perpendicular lines that pass through that location appear as well. The Extended Cross Hairs option displays perpendicular lines that pass through the cursor location and extension lines that connect those lines to the axes. These cursor styles are shown below.



Wireframe planes



Extended cross hairs

Selecting a navigation mode

The Navigation Mode options let you specify a method for manipulating the 3-D image. The table below describes the available options.

Option	How to Manipulate the 3-D Image
Rotate	To rotate the image, drag an edge or corner as though you were swinging that point around the center of the image. If you release the mouse button while dragging the point, the image continues to move in an "animated rotation." To stop this rotation, click the image.
Combined	In addition to the manipulation techniques described for the Rotate option, you can drag vertically across the image with the *right* mouse button held down to enlarge or shrink the image. You can also hold down the Shift key and drag the image in any direction to move it within the pane (as you can with the Pan option).
Zoom	To enlarge or shrink the image, drag vertically across it.
Pan	Drag the image in any direction to move it within the pane.

In all modes you can enlarge or shrink the image by pointing at it and turning the mouse wheel (if present).

Note You can also specify a navigation mode by *right-clicking* the 3-D image, pointing to Navigation Mode and choosing a mode from the pop-up menu. ▲

Displaying the 3-D image in perspective

Perspective

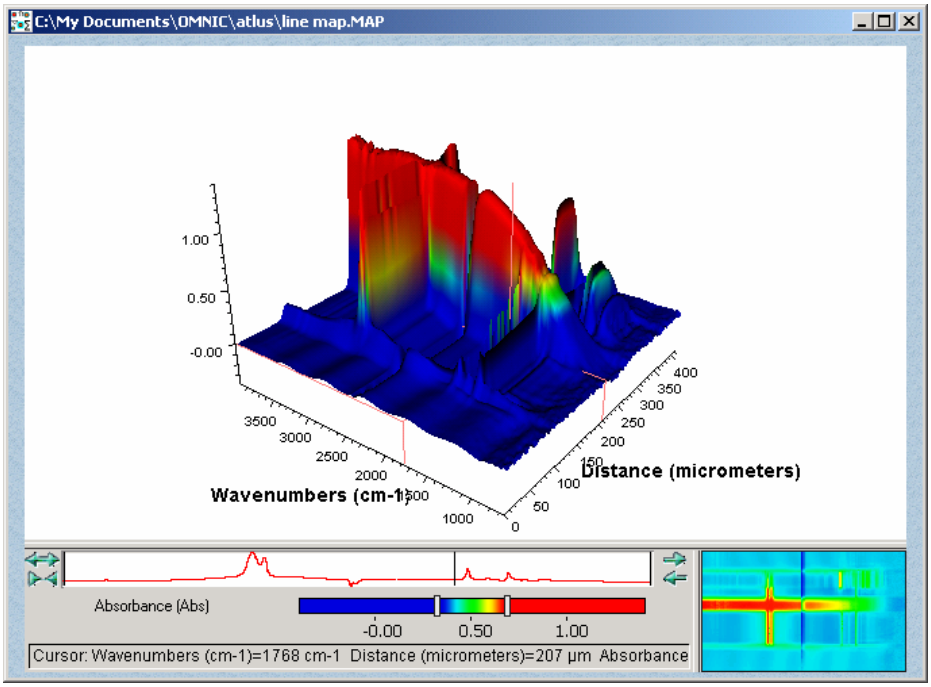
Select Perspective if you want the 3-D image displayed in perspective (with foreshortening that creates the illusion of depth).

Clipping the data outside the color range

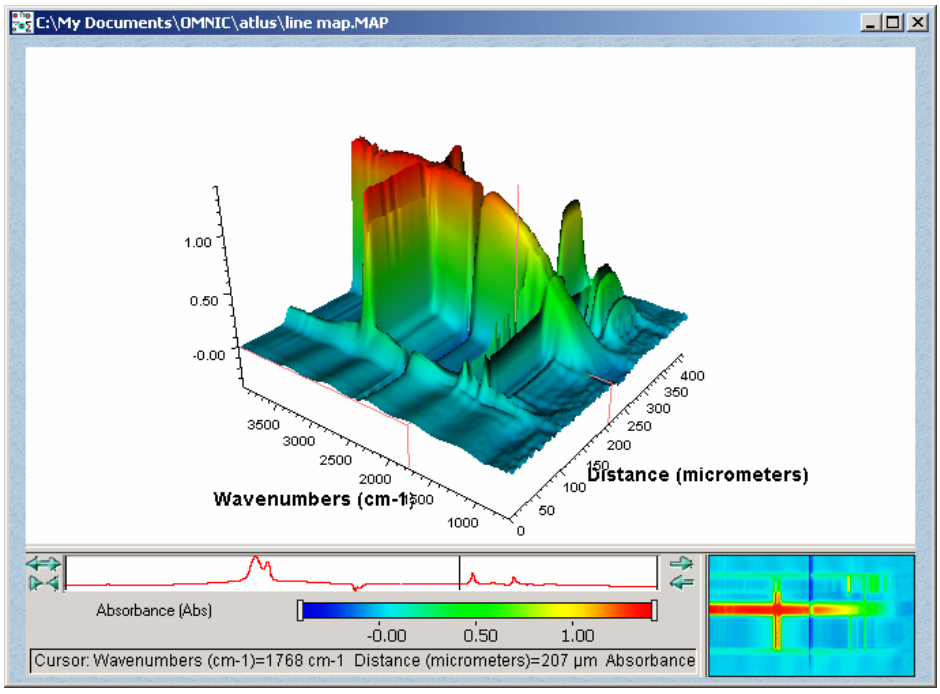
Clip data outside color range

Select Clip Data Outside Color Range if you want data outside the spectral intensity range specified by the color bar not to be displayed in the 3-D image. (This option does not effect the 3-D image if Show Full Volume is selected.) This results in the display of only the data in the intensity range of interest.

The illustrations below show a 3-D image before and after being clipped. Note that the spectral intensity range specified by the color bar in the first illustration is narrower than the full intensity range of the map data. This lets you see more color gradations, and thus more detail, in the intensity range of interest. In the second illustration the new color bar range matches the narrowed spectral intensity range.



3-D image before clipping

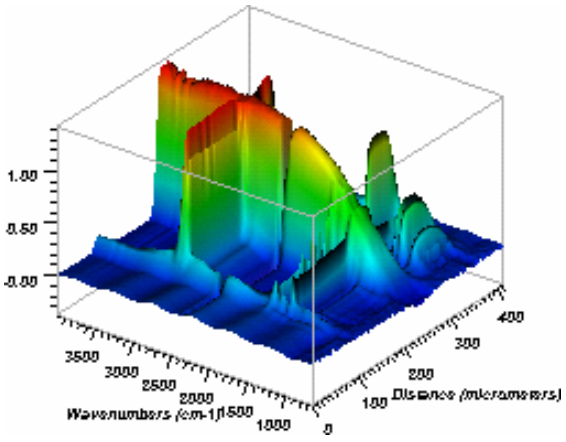


Clipped 3-D image

Displaying an outline box

Show outline box

Select Show Outline Box if you want the outer limits of the 3-D image to be indicated by lines that form a bounding box around the image. Here is an example:

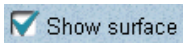


Displaying the map title above the 3-D image

Show title

Select Show Title if you want to display the map title above the 3-D image in a map window, or the profile type above the 3-D image in a profile window. You can change the title by using Show Map Info in the Atlµs menu. See “Viewing information about a map” for more information.

Displaying surfaces in the 3-D image



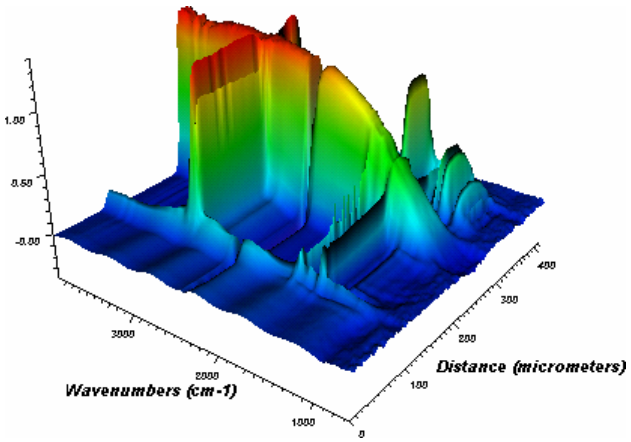
Select Show Surface if you want to display map data in the form of a 3-D image that appears as a surface plot (a warped, interpolated surface).

For a line map (or line depth profile) each point on the surface of the plot represents the spectral intensity value at a particular frequency and distance along the line on the sample (or within the sample).

For an area map (or area depth profile) each point on the surface represents the value of the specified type at an X-Y location on the sample (or X-Z location within the sample).

Here is an example showing the 3-D image of a line map:

You can also specify this type of display by *right-clicking* the 3-D image, pointing to 3-D Display and choosing Show Surface from the pop-up menu.



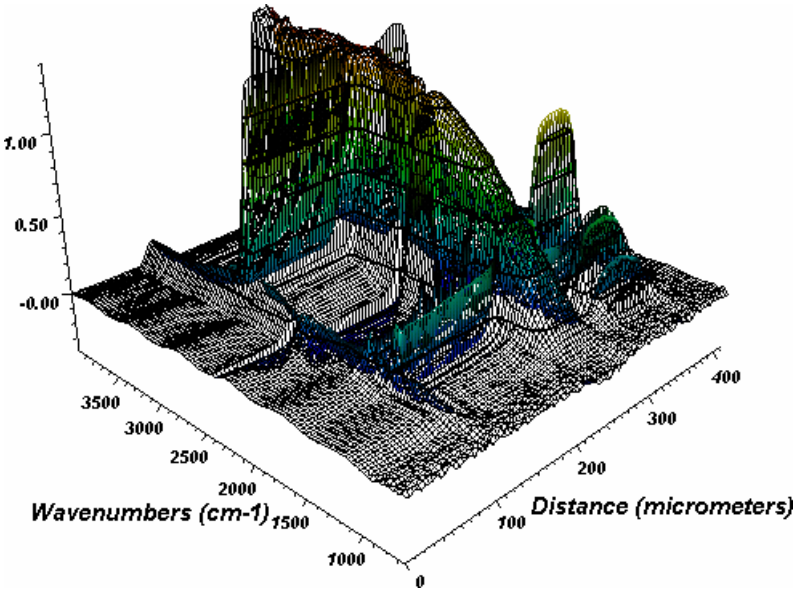
3-D image of two-dimensional data displayed as a surface plot

Note You cannot select both Show Surface and Profile Lines. See "Displaying profile lines in the 3-D image" for information about using Profile Lines. ▲

Displaying the 3-D image as a wireframe

Select Wireframe if you want to display map data in the form of a 3-D image that appears as a wireframe surface plot, with lines connecting points having the same vertical-axis value. This is similar to the surface plot displayed by the Show Surface option, except gaps appear between the wireframe lines. (If you are displaying an area map or area depth profile and have selected both Wireframe and Show Surface, the wireframe is overlaid on the surface plot.) See "Displaying surfaces in the 3-D image" for more information.

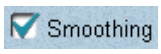
Here is an example showing the 3-D image of a line map:



3-D image of two-dimensional data displayed as a wireframe surface plot

Note If you are displaying an area map or area depth profile, Wireframe is available only if you have not selected Show Full Volume. See "Displaying the full volume of the 3-D image" for information about using Show Full Volume. ▲

Smoothing the 3-D image



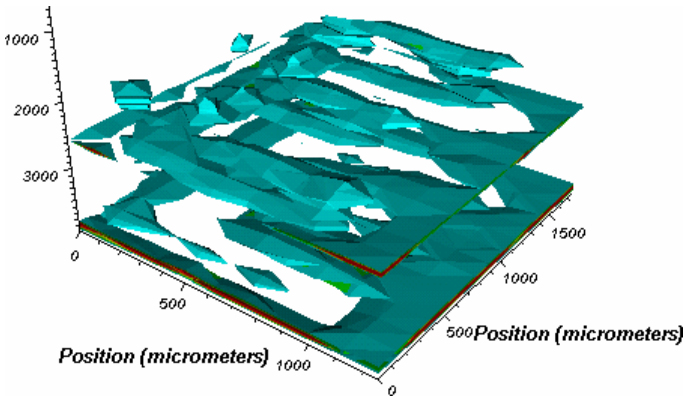
Select Smoothing if you want the 3-D image to have smoother edges and more blended color transitions.

Displaying the full volume of the 3-D image

If you are displaying an area map or area depth profile, you can select Show Full Volume to display the full volume of the three-dimensional data, using iso-surfaces that are similar to two-dimensional contour lines. This shows where the volume data crosses intensity grade value thresholds. The setting of Number Of Iso-surfaces determines the number of grades (iso-surfaces) to display. See "Setting the number of iso-surfaces or contours to display" for more information.

In the example below, the X position and Y position on the microscope stage are indicated by the two Position axes and frequency is indicated by the vertical axis. Values (such as spectral intensity) are indicated by colors, as specified by the color bar.

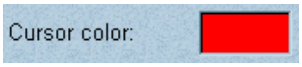
You can also specify this type of display by *right-clicking* the 3-D image, pointing to 3-D Display and choosing Show Full Volume from the pop-up menu.



Full volume displayed in 3-D image

Note If you select Show Full Volume, Wireframe is not available. See "Displaying the 3-D image as a wireframe" for information about using Wireframe. ▲

Specifying a color for the 3-D image cursor



The color in the box to the right of Cursor Color shows the color used to display the 3-D image cursor. To change the color, click the box. The Color dialog box (a Windows feature) appears allowing you to select a color. If you need help using the features in this dialog box, click the "?" button and then click the feature of interest. When you are finished selecting a color, choose OK.

Hiding the 3-D image cursor

If you want to hide the cursor for the 3-D image, select Hide Cursor.

Setting the number of iso-surfaces or contours to display

If Show Full Volume is selected, the Number Of Iso-surfaces parameter is available. Specify the number of iso-surfaces to display in the 3-D image by typing a number in the Number Of Iso-surfaces text box or by clicking the up and down arrows to the right of the text box. An iso-surface is an intensity value grade, a generalization of the two-dimensional contour line. It shows where the volume data crosses an intensity grade value threshold.

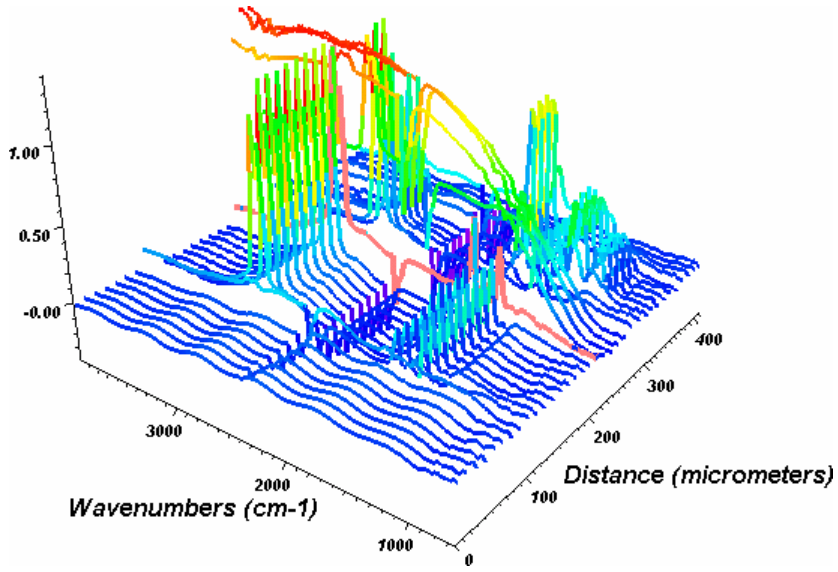
If Show Full Volume is not selected, the Number Of Contours parameter is available. Specify the number of contours to display in the 3-D image by typing a number in the Number Of Contours text box or by clicking the up and down arrows to the right of the text box.

See “Displaying the full volume of the 3-D image” for information about using Show Full Volume.

Displaying profile lines in the 3-D image

Profile lines

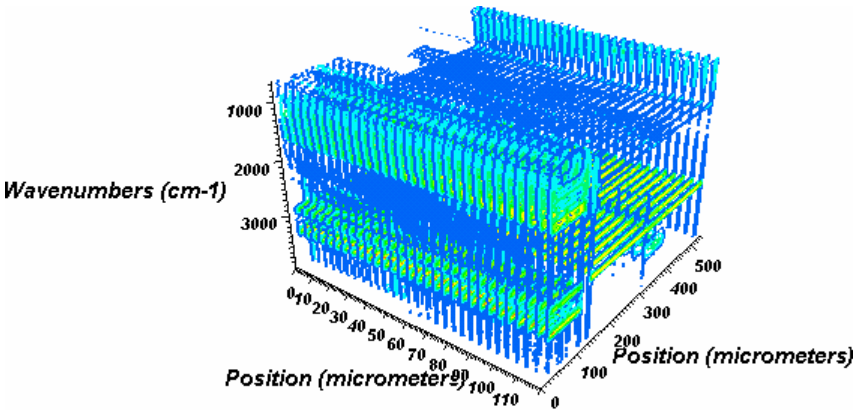
Select Profile Lines if you want profile lines representing values of constant grade to appear in the 3-D image. This gives the image the appearance of having been sliced with equally spaced imaginary planes. Here is an example showing a line map with the profile lines in the X-Z plane:



3-D image of line map data with profile lines

Use Profile Orientation to specify the orientation of the lines; that is, in which plane the lines lie. Use Number Of Profiles to set the number of profile lines. See “Specifying the orientation of the profile lines” for information about using Profile Options. See “Setting the number of profile lines in the 3-D image” for information about using Number Of Profiles.

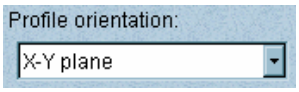
The illustration below shows an example of the 3-D image of an area map with Show Full Volume selected. The colors of the profile lines indicate value. See “Displaying the full volume of the 3-D image” for information about using Show Full Volume.



3-D image of area map data showing full volume

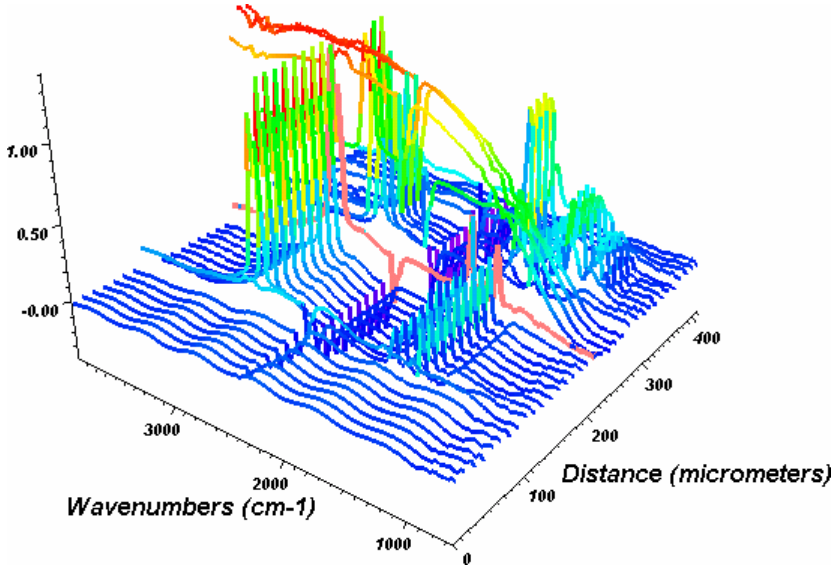
Note You cannot select both Show Surface and Profile Lines. See “Displaying surfaces in the 3-D image” for information about using Show Surface. ▲

Specifying the orientation of the profile lines

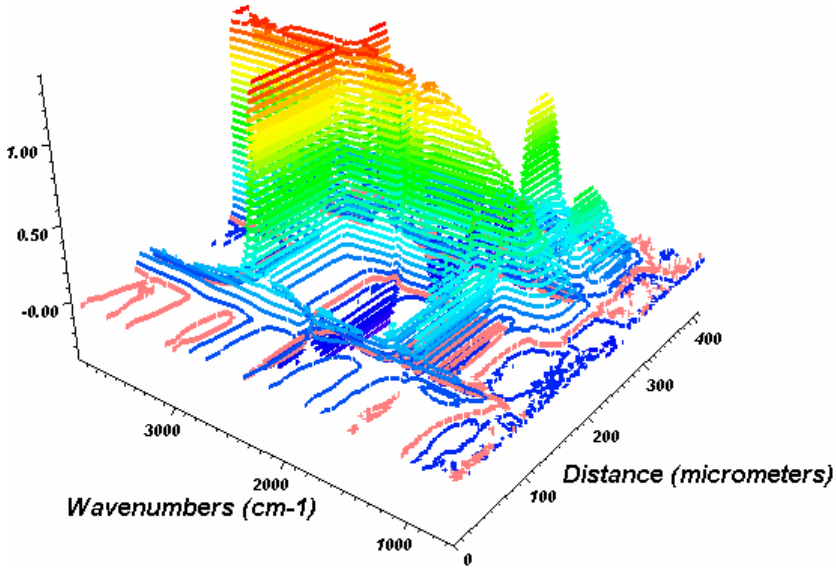


If you have selected Profile Lines to display profile lines in the 3-D image, specify the orientation of the lines by setting Profile Orientation. The following illustrations show the available orientations: X-Z Plane, X-Y Plane and Y-Z Plane. Use Number Of Profiles to specify how many profile lines appear in the image. See “Displaying profile lines in the 3-D image” for information about using Profile Lines. See “Setting the number of profile lines in the 3-D image” for information about using Number Of Profiles.

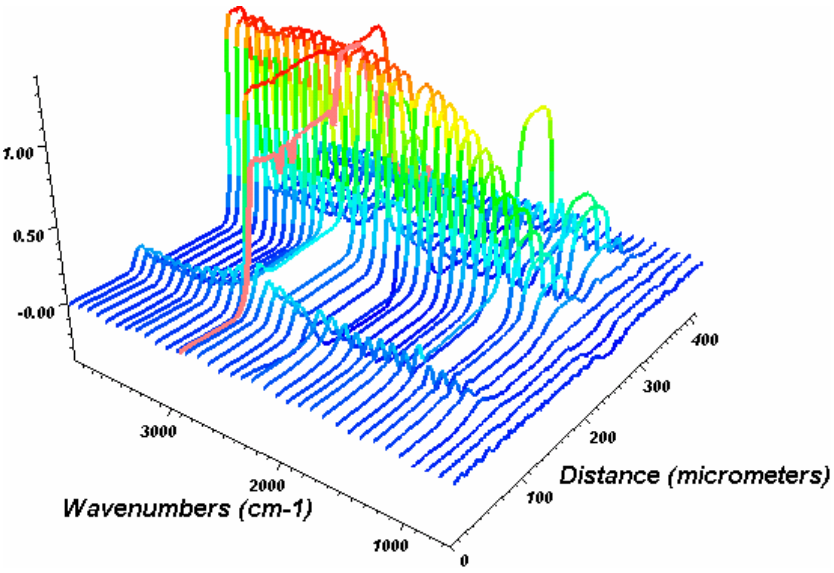
Note If profile lines with X-Y orientation were projected onto the same horizontal plane, the lines would match the contour lines in the contour map, if displayed. ▲



Profile lines with X-Z orientation

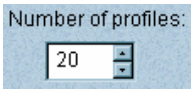


Profile lines with X-Y orientation



Profile lines with Y-Z orientation

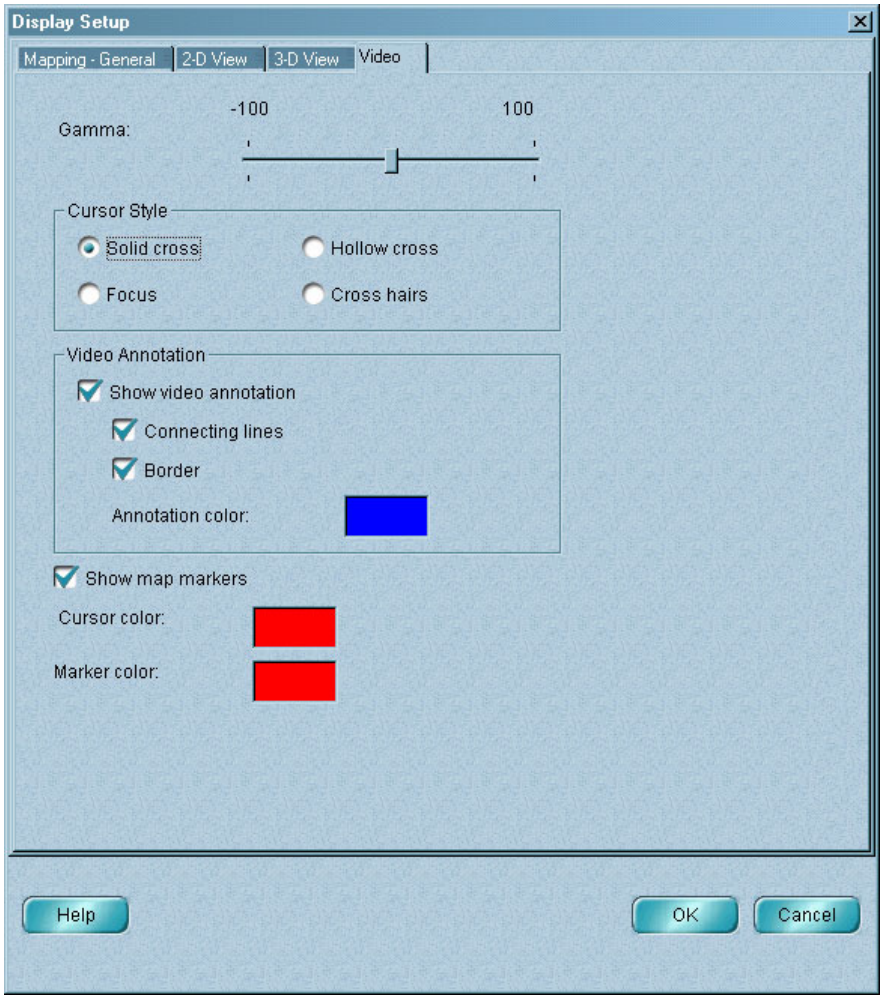
Setting the number of profile lines in the 3-D image



If you have selected Profile Lines to display profile lines in the 3-D image, specify the number of lines by typing a number in the Number Of Profiles text box or by clicking the up and down arrows to the right of the text box. Use Profile Orientation to specify the orientation of the lines (in which plane the lines lie). See “Displaying profile lines in the 3-D image” for information about using Profile Lines. See “Specifying the orientation of the profile lines” for information about using Profile Orientation.

Video display parameters

The video display parameters appear on the Video tab:

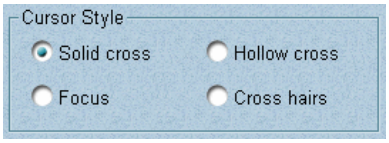


The next sections explain how to use these features.

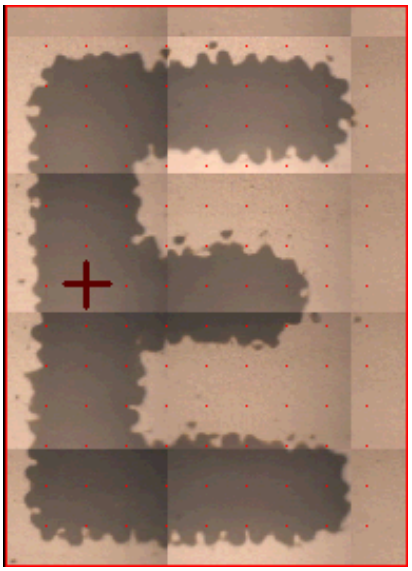
Changing the brightness and contrast

Use Gamma to improve the appearance of the video image. (The term "gamma" refers to part of a mathematical expression relating the input and output signals of a display device.) Drag the vertical bar to the right to increase brightness and reduce contrast; drag the bar to the left to reduce brightness and increase contrast.

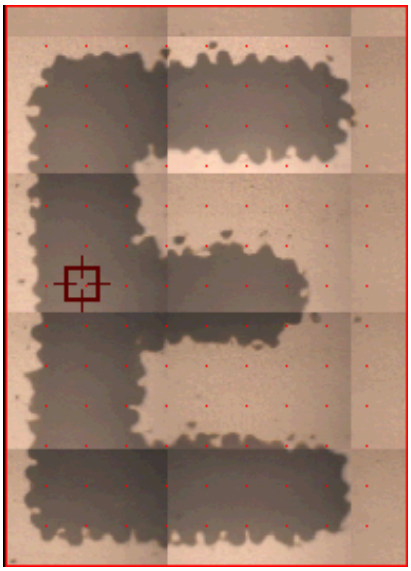
Selecting a cursor style for the video image



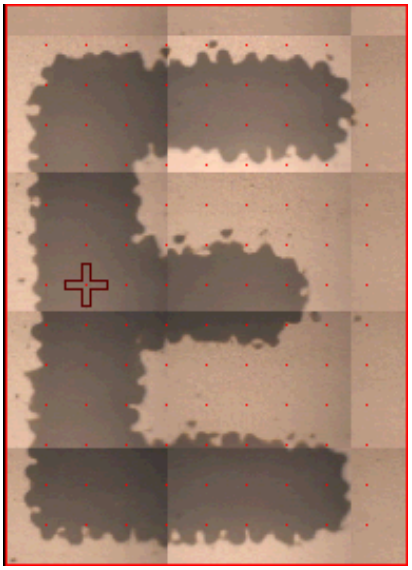
Specify a cursor style for the video image by selecting an option in the Cursor Style box. The available styles are shown below.



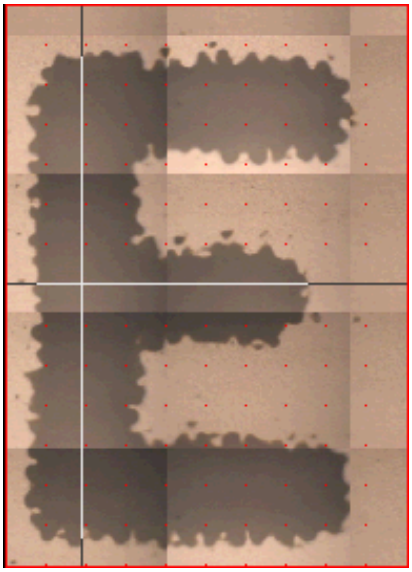
Solid Cross



Focus

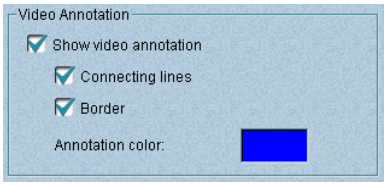


Hollow Cross



Cross Hairs

Setting the video annotation parameters



If you want annotation to be visible in the video image, select Show Video Annotation. This allows you to set the other parameters in the Video Annotation box.

If you want the connecting lines for text annotation to appear in the video image, select Connecting Lines. See "Connecting text annotation with a line" and "Adding text annotation" in the "Preparing for Data Collection" chapter for information about creating text annotation that is connected with lines.

If you want the border of text annotation to appear in the video image, select Border. See "Displaying a border around text annotation" for more information.

To change the color of displayed video annotation, click the Annotation Color box. The Color dialog box (a Windows feature) lets you select a color. If you need help using the features in this dialog box, click the "?" button and then click the feature of interest. When you are finished selecting a color, choose OK.

Displaying markers

Select Show Map Markers if you want markers added with the marker tool to appear in the video image. You can also toggle the display of markers by *right-clicking* the video image and choosing Show Markers from the pop-up menu. See "Adding a marker" in the "Preparing for Data Collection" chapter for information about adding markers.

Specifying colors for the video image cursor and markers

The color in the box to the right of Cursor Color shows the color used to display the video image cursor. To change the color, click the box. The Color dialog box (a Windows feature) appears allowing you to select a color. If you need help using the features in this dialog box, click the "?" button and then click the feature of interest. When you are finished selecting a color, choose OK.

The color in the box to the right of Marker Color shows the color used to display markers in the video image. To change the color, use the same technique as described above for the cursor color. For more information about markers, see "Adding a marker" in the "Preparing for Data Collection" chapter.

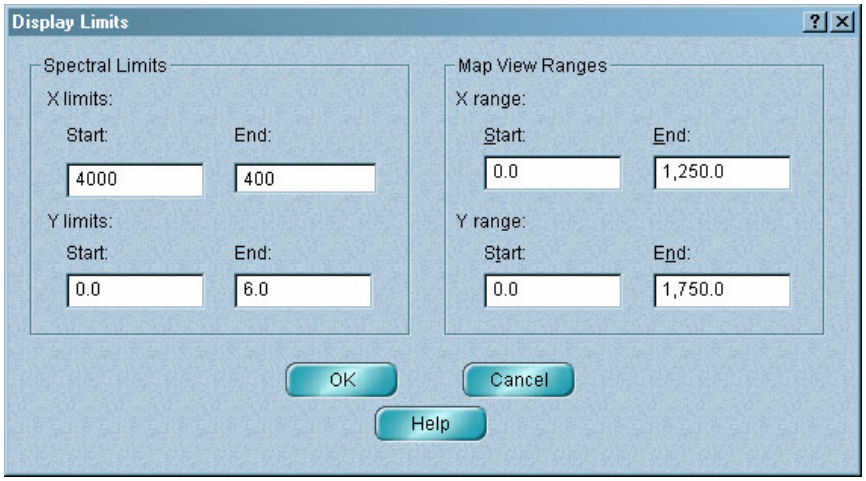
Setting the display limits

Use Display Limits in the View menu to specify the axis display limits for data in the active map window or profile window. Follow these steps:

1. **Choose Display Limits from the View menu.**

   The Display Limits dialog box appears:

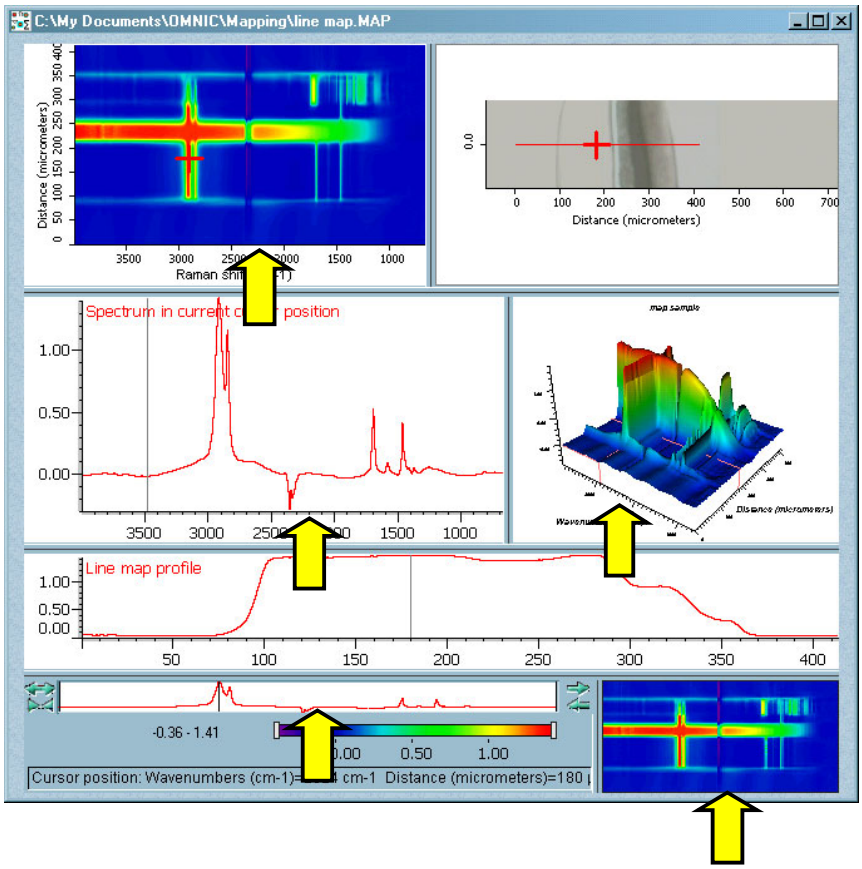
The X Range and Y Range features in the Map View Ranges box are available only for area maps. The Map View Ranges features are not available for discrete point maps.



2. **Type the desired frequency limits in the X Limits Start and End text boxes in the Spectral Limits box.**

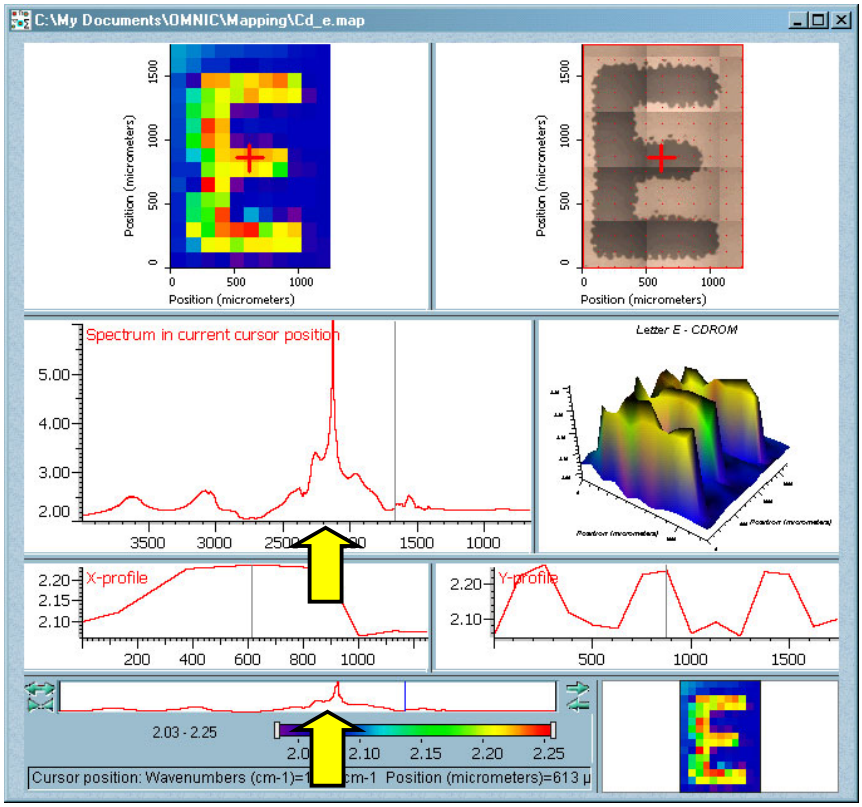
Note You can also use the view finder to change the frequency limits. See "Using map window" for details. ▲

For a line map (or line depth profile) this sets the display limits for the frequency axes of the contour map (and corresponding area of the sky view control), spectral display pane, 3-D image and white area of the view finder, as indicated by the arrows in the illustration below:



Line map (and line depth profile) frequency axes

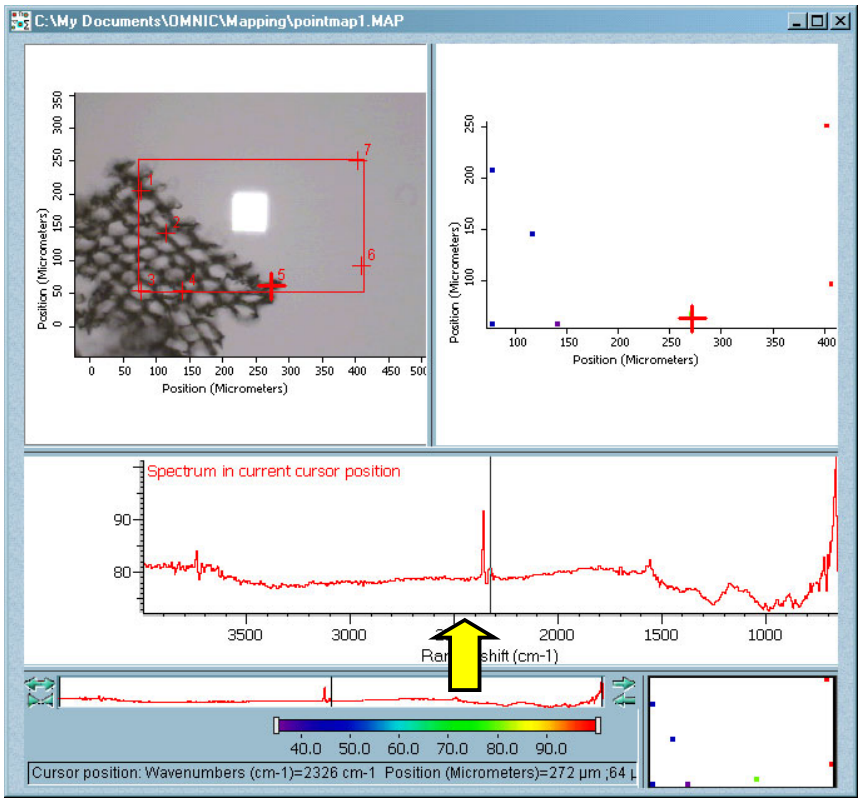
For an area map (or area depth profile) this sets the display limits for the X-axis of the spectral display pane and white area of the view finder, as indicated below:



Area map (and area depth profile) frequency axis

Note If you have selected Show Full Volume on the 3-D View tab of the Display Setup dialog box, the entered frequency limits also determine the spectral range of area map (or area depth profile) data that is visible in the 3-D image, without changing the limits of the image's vertical axis. See "Displaying the full volume of the 3-D image" for information about using Show Full Volume. ▲

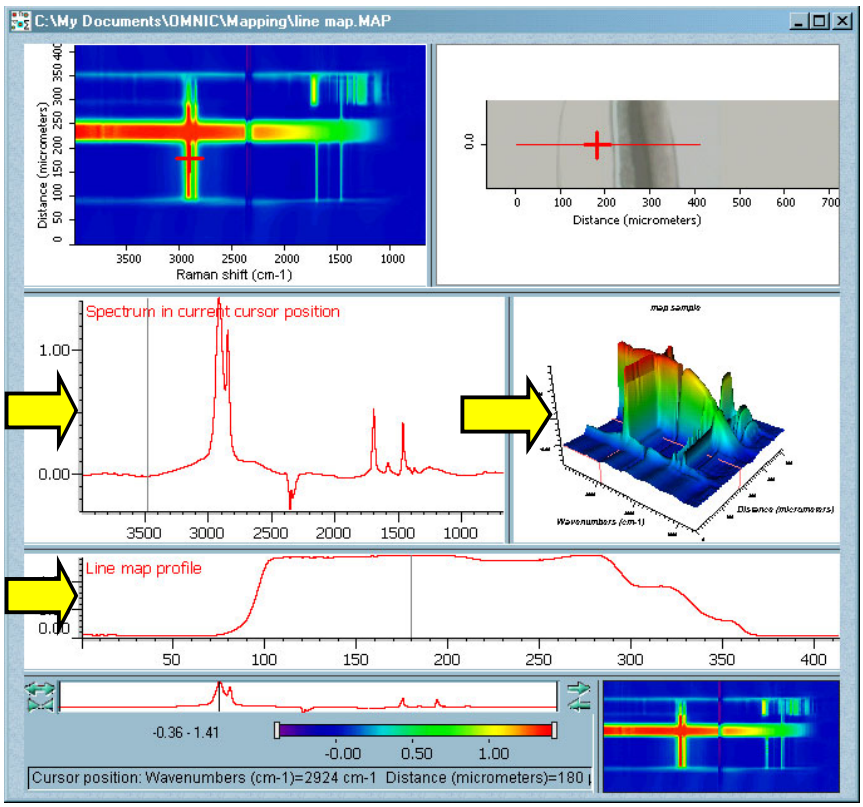
For a discrete point map this sets the display limits for the X-axis of the spectral display pane, as indicated below:



Discrete point map frequency axis

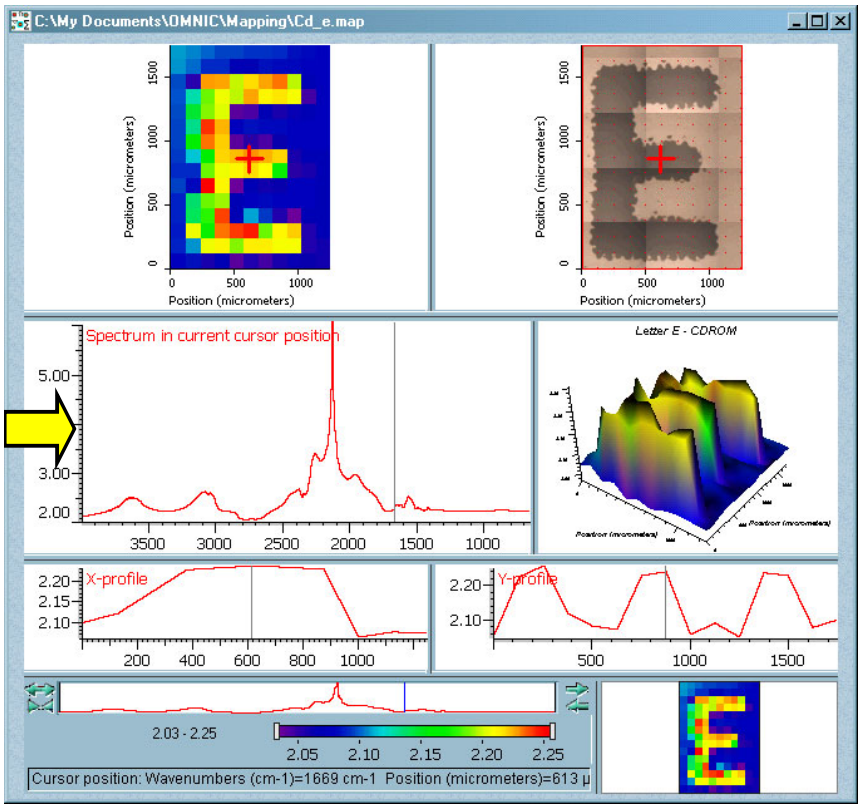
3. **Type the desired spectral intensity limits in the Y Limits Start and End text boxes in the Spectral Limits box.**

   For a line map (or line depth profile) this sets the display limits for the vertical axis of the spectral display pane, 3-D image and profile pane, as indicated below:



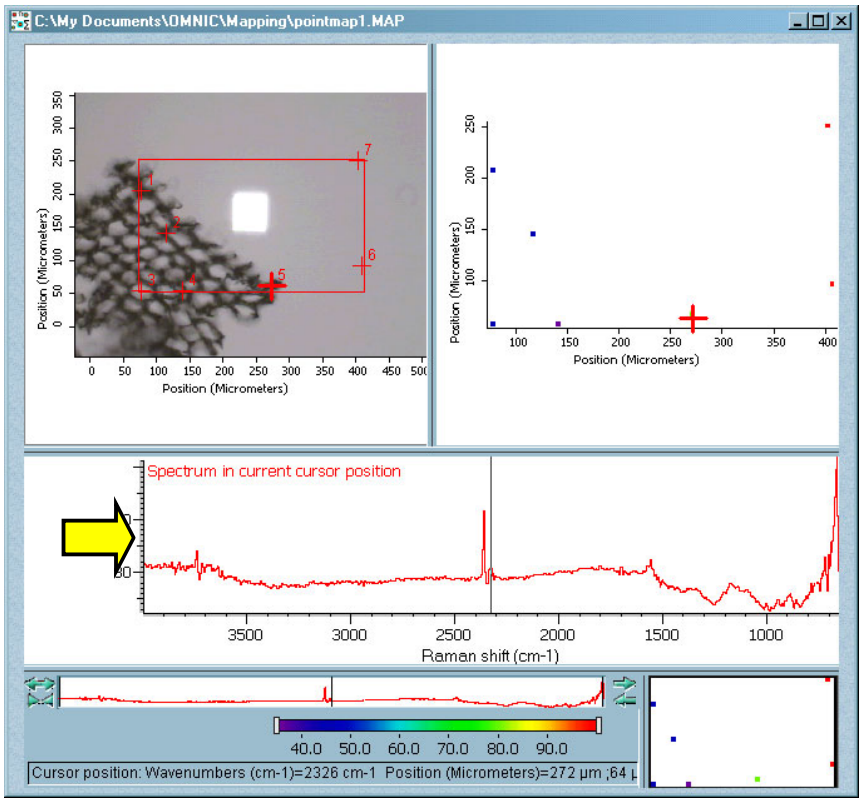
Line map (and depth profile) spectral intensity axes

For an area map (or area depth profile) this sets the display limits for the Y-axis of the spectral display pane, as indicated below:



Area map (and area depth profile) spectral intensity axis

For a discrete point map this sets the display limits for the Y-axis of the spectral display pane, as indicated below:



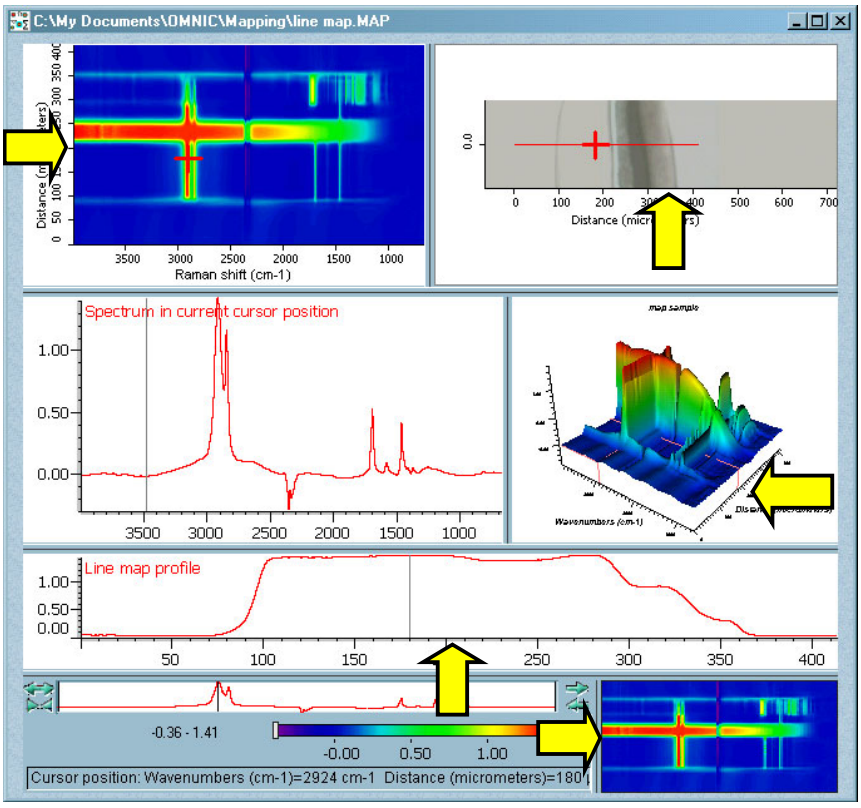
Discrete point map spectral intensity axis

4. **If you are setting the display limits for a discrete point map, choose OK; the procedure is finished.**

   For a line map or line depth profile, type the distance limits in the Distance Start and End text boxes in the Map View Ranges box.

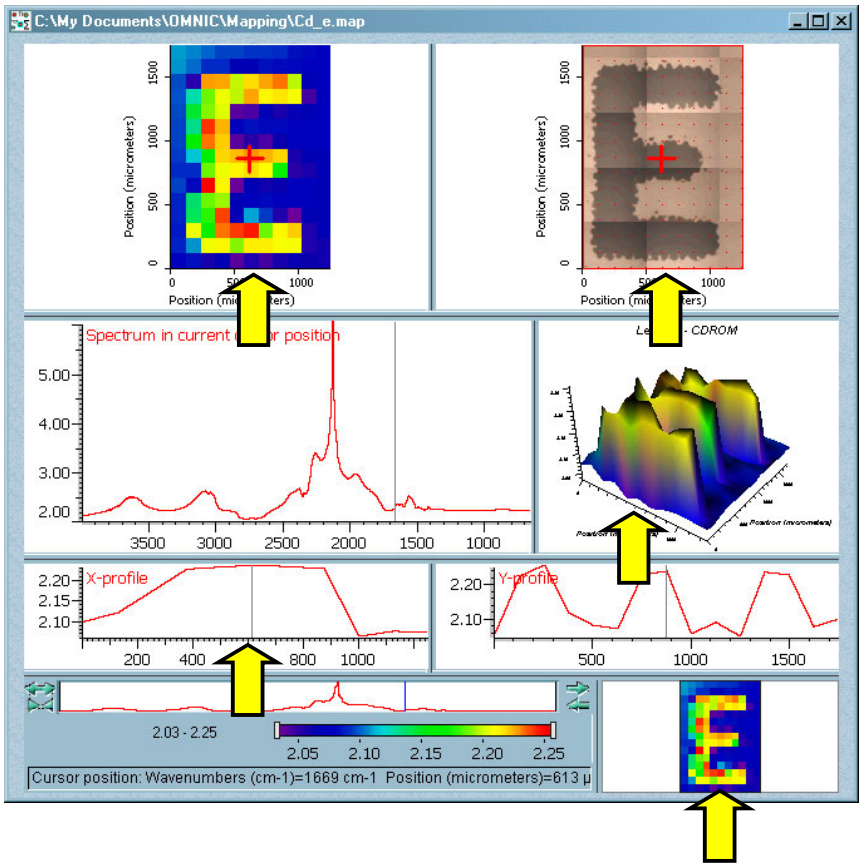
   For an area map or area depth profile, type the X distance limits in the X Range Start and End text boxes in the Map View Ranges box.

For a line map (or line depth profile) this sets the display limits for the distance axis of the contour map (and corresponding area of the sky view control), video image, 3-D image and profile pane, as indicated below:



Line map (or depth profile) Y (or Z) spatial axes

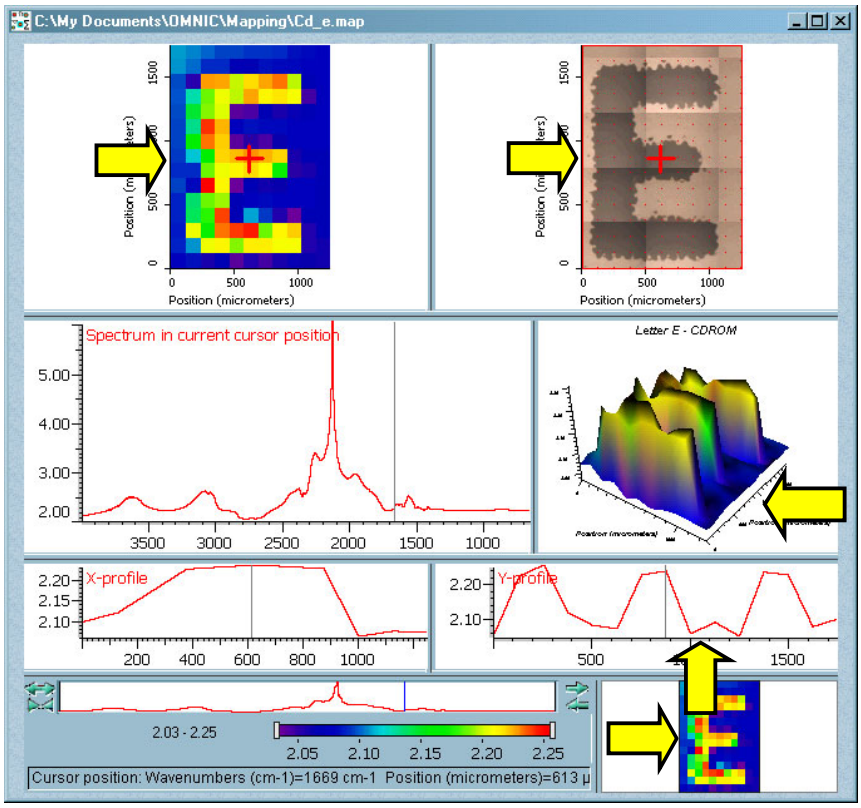
For an area map (or area depth profile) this sets the display limits for the X distance axis of the contour map (and corresponding area of the sky view control), video image, 3-D image and X-profile pane, as indicated below:



Area map (and area profile) X spatial axes

5. **If you are setting the display limits for a line map or line depth profile, choose OK; the procedure is finished. If you are setting the limits for an area map or area depth profile, type the Y (or Z) distance limits in the Y Range Start and End text boxes in the Map View Ranges box.**

   This sets the display limits for the Y (or Z) distance axis of the contour map (and corresponding area of the sky view control), video image, 3-D image and Y-profile pane, as indicated below:



   Area map (or area depth profile) Y (or Z) spatial axes

6. **Choose OK.**

Displaying the current profile or a saved profile

If you are displaying an area map or area depth profile, you can use Show Current Profile in the Atlμs menu to display a profile that was created during map data collection or created and saved after collection. You can then manipulate the display of the data (for example, by using Display Setup in the View menu). You cannot process the data using the Process menu commands.

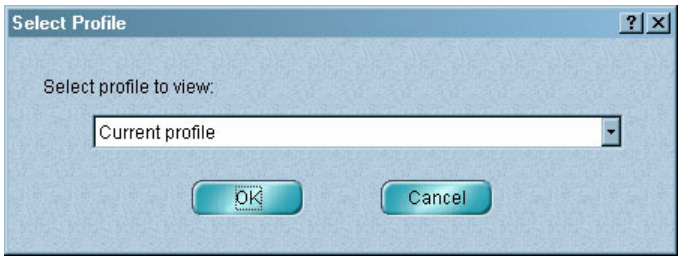
Profiles are displayed in a profile window, which is very similar to a map window. See "Using map windows" for information about manipulating the parts of the window. To close the window, click the Close button (labeled "X") in the upper-right corner.

If a map window is displayed, you can use Profile Setup in the Atlμs menu to create a new profile and save it with the map. See "Creating a profile" in the "Processing and Analyzing Map Data" chapter for details.

Follow these steps to display a profile:

1. **Choose Show Current Profile from the Atlμs menu.**

   If you have not saved multiple profiles with the map, the current profile appears in a profile window and the procedure is finished. If multiple profiles have been saved, the Select Profile dialog box appears:



2. **Select the desired profile from the drop-down list box.**

3. **Choose OK.**

   The profile appears in a profile window.

Overlaying the video image and contour map or discrete point location map

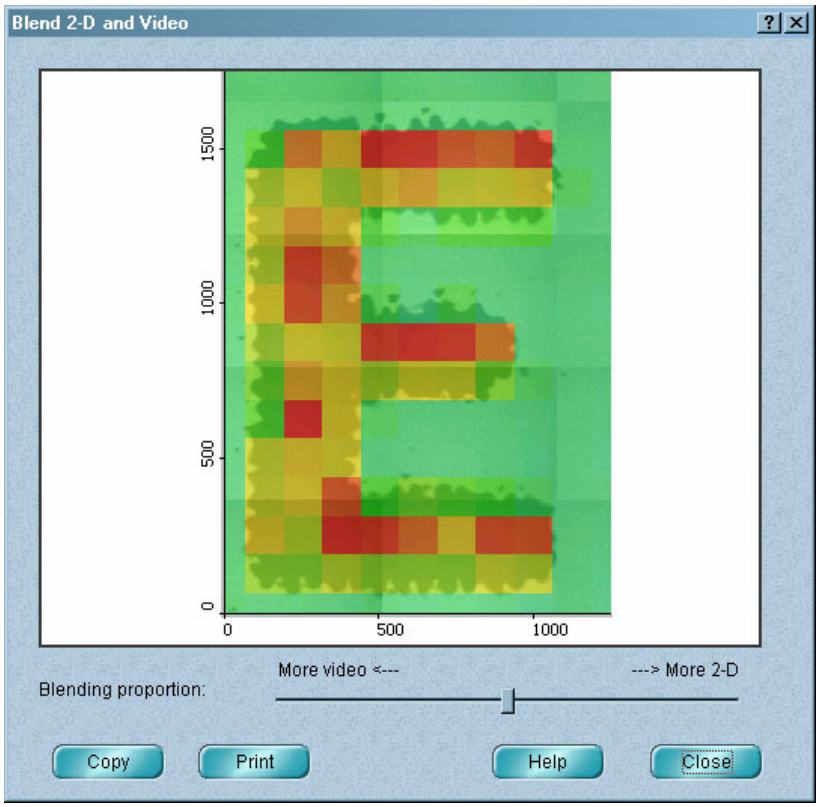
Use Blend 2-D And Video in the Atlμs menu to view an image formed by overlaying the contour map or discrete point location map and video image displayed in the active map window. This makes it easy to see spatial relationships between map and video image features.

Note You cannot overlay the video image for a depth profile. ▲

Follow these steps:

1. **Choose Blend 2-D And Video from the Atlμs menu.**

   The Blend 2-D And Video window appears:



   The map and video image appear overlaid, with reduced opacity. This lets you see features of both.

   By dragging the vertical bar along the Blending Proportion control, you can adjust the contribution each image makes to the overlaid image.

You can zoom in on an area of interest by using the mouse to draw a box around the area and then clicking inside the box. If desired, drag the handles on the sides or corners of the box to adjust its size and shape before clicking inside it. To return the overlaid image to its original size, double-click it.

You can copy the blended image to the Windows Clipboard by clicking the Copy button. You can then paste the image using another Windows application that uses the Clipboard.

You can print the blended image by clicking the Print button.

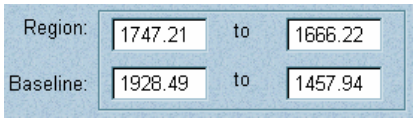
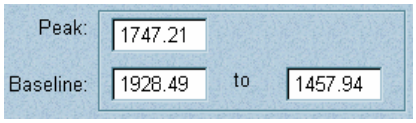
2. **To close the window, click the Close button.**

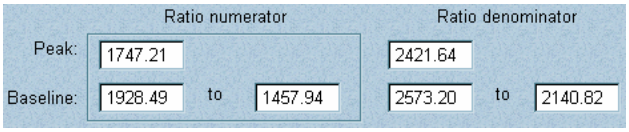
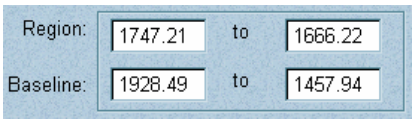
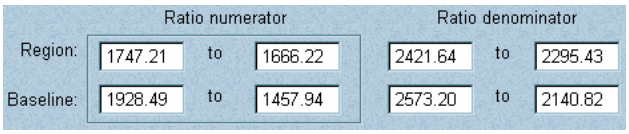
Processing and Analyzing Map Data

This chapter explains how to process map data displayed in a map window. After you have processed a map, you can save your changes with Save Map or Save Map As in the File menu. See the "Saving and Exporting Map Data" chapter for complete information.

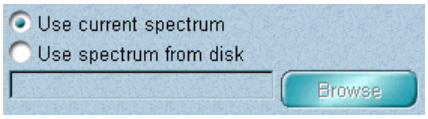
Creating a profile

Use Profile Setup in the Atlμs menu to create a new profile from a line map, area map or depth profile displayed in the active map window. The term "profile" is used to refer to any of the ways of representing map data described in the table below and in the next section. The table also describes the information you need to specify for each profile type. The numerical values shown are just examples.

Profile Type	What the Profile Shows	Needed Information
Chemigram	The integrated spectral intensity of a specified spectral region for each sample point.	The frequency limits of the spectral region and baseline endpoints:  Profiles created using the Chemigram and Peak Area Of One Peak profile types are identical.
Peak Height Of One Peak	The corrected height of the specified peak for each sample point.	The frequency location of the peak and the baseline endpoints: 

Profile Type	What the Profile Shows	Needed Information
Peak Height Ratio Of Two Peaks	The ratio of the corrected heights of two specified peaks for each sample point.	The frequency locations of the two peaks and their baseline endpoints:  The parameters for the peak whose height will be the numerator in the ratio are labeled “Ratio Numerator”; the parameters for the denominator peak are labeled “Ratio Denominator.”
Peak Area Of One Peak	The corrected area of the specified peak for each sample point.	The frequency limits of the peak and baseline endpoints:  Profiles created using the Chemigram and Peak Area Of One Peak profile types are identical.
Peak Area Ratio Of Two Peaks	The ratio of the corrected areas of two specified peaks for each sample point.	The spectral regions of the two peaks and their baseline endpoints:  The parameters for the peak whose area will be the numerator in the ratio are labeled “Ratio Numerator”; the parameters for the denominator peak are labeled “Ratio Denominator.”

Profile Type	What the Profile Shows	Needed Information
Functional Group	The correlation between the integrated spectral intensities of the map spectra and the weighted intensities of the selected functional group within the spectral regions specified for the group. This lets you quickly find the locations on the sample where absorptions most characteristic of the functional group occurred. *Turn off Auto Threshold and set Background Threshold to 0 and Foreground Threshold to 1 in the Display Setup dialog box before creating this profile type.* See "Setting the thresholds automatically" and "Specifying the background and foreground thresholds" in the "Displaying Map Data" chapter for more information.	The identity of the functional group. To specify a predefined functional group (a set of more than fifty functional groups is provided with the software), select the Predefined Groups option and then select a group from the Functional Group drop-down list box and a type from the Type drop-down list box. The available types depend on the functional group you have selected.  To specify a functional group you have defined using Edit Functional Groups in the Atlμs menu, select the User-Defined option and then select a group from the Functional Group drop-down list box. (The Type drop-down list box is not available for user-defined groups.)  See "Viewing, editing or creating functional groups" in the "Processing and Analyzing Map Data" chapter for details on defining your own functional groups.

Profile Type	What the Profile Shows	Needed Information
Correlation Map	The correlation between the map spectra and the specified reference spectrum. This lets you find the locations of the reference compound (or similar compounds) on the sample. The resulting correlation intensity values of the map spectra are analogous to the match values of library spectra displayed after a spectral search. A higher intensity value indicates a greater similarity to the reference spectrum. A value of 1.0 indicates that the map spectrum and reference spectrum are identical. *Turn off Auto Threshold and set Background Threshold to 0 and Foreground Threshold to 1 in the Display Setup dialog box before creating this profile type.* See "Setting the thresholds automatically" and "Specifying the background and foreground thresholds" in the "Displaying Map Data" chapter for more information.	The spectrum to use as the reference:  If you want to use the spectrum in the spectral display pane, select Use Current Spectrum. If you select Use Spectrum From Disk, type the pathname of the desired spectrum in the text box, or use the Browse button to locate and select a spectrum.

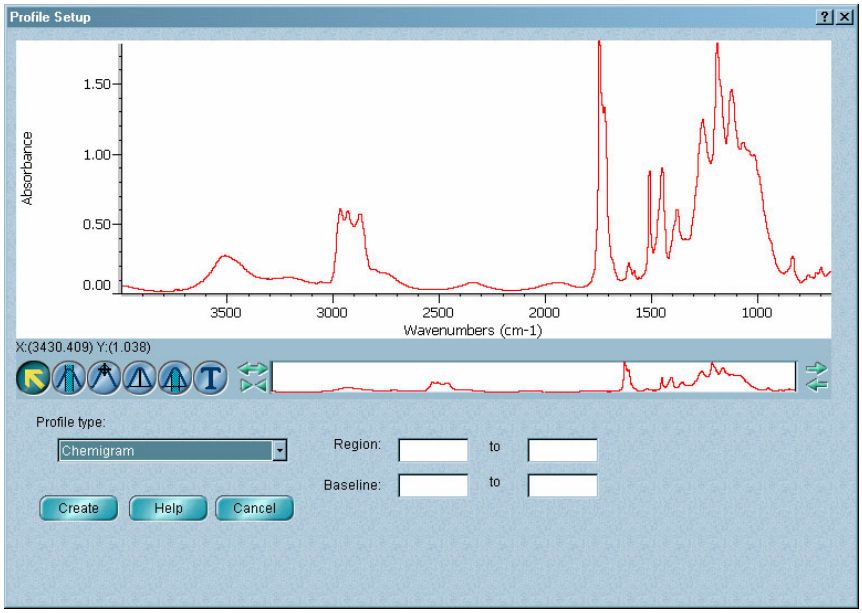
Note Profiles created using the Chemigram and Peak Area Of One Peak profile types are identical. ▲

In each case a profile created from a map is displayed in a profile window, which closely resembles a map window.

Follow these steps to create a profile using the line map or area map displayed in the active map window:

1. **Choose Profile Setup from the Atlµs menu.**

   The Profile Setup window appears:



2. **Set Profile Type to the desired profile type.**

   Depending on the type you select, text boxes, a drop-down list box or option buttons may appear allowing you to enter or select the needed information. See the table earlier in this section for a description of these items.

3. **Enter or select the appropriate information.**

   You can use the palette tools to specify some information graphically within the spectral display pane.

   - If you are creating a Chemigram, use the region tool or peak area tool to select a spectral region. See “Selecting a spectral region” or “Specifying peak areas and baselines” if you are not familiar with using the tools.

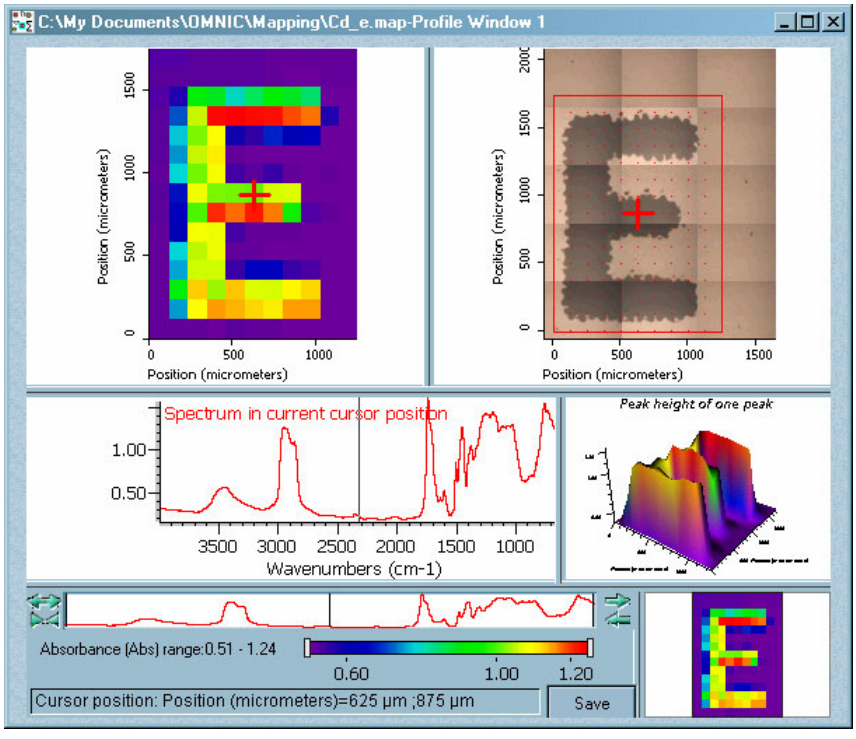
- If you selected the Peak Height Of One Peak or Peak Height Ratio Of Two Peaks options, use the peak height tool to specify the peak or peaks and a baseline. See “Specifying peak locations and baselines” for complete information.

- If you selected the Peak Area Of One Peak or Peak Area Ratio Of Two Peaks options, use the peak area tool to specify the peak or peaks and a baseline. (You can also use the region tool if you don’t need to manipulate the baseline endpoints graphically.) See “Specifying peak areas and baselines” for details on using the peak area tool. See “Selecting a spectral region” for information on using the region tool.

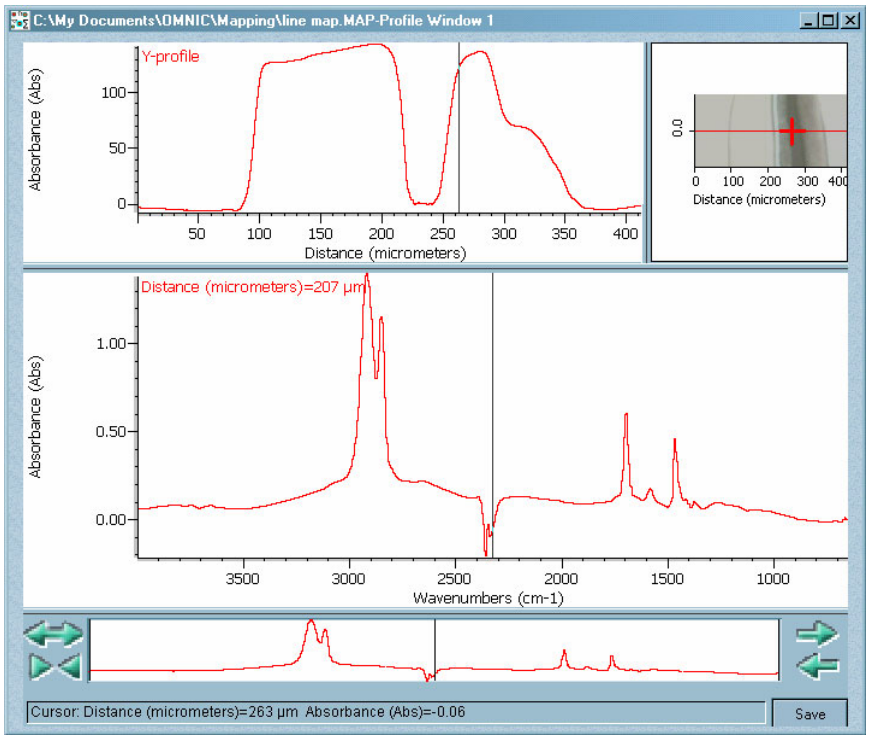
You can change the displayed spectral region by using the view finder below the spectral display pane. See the OMNIC Help system if you need information on using the view finder.

4. Click the Create button to create the new profile.

The new profile appears in a profile window. Below is an example showing a profile created from an area map. A profile created from an area depth profile would be similar.



Below is an example showing a profile created from a line map. A profile created from a line depth profile would be similar.

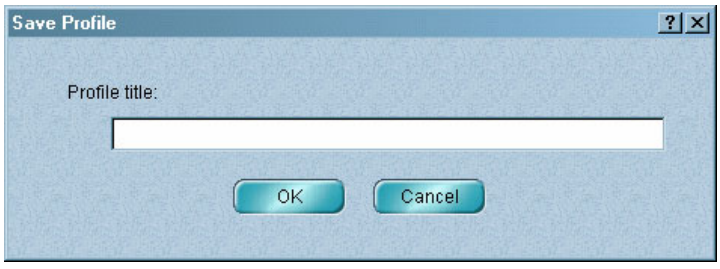


You can use Display Setup in the View menu to change how data is displayed just as you would for a map window. See “Setting the display parameters” in the “Displaying Map Data” chapter for details.

If you don’t want to save the profile, the procedure is finished.

5. To save the profile, click the Save button.

The Save Profile dialog box appears:



6. Type a title for the profile in the text box.

7. **Choose OK.**

   You can open the profile later by using Show Current Profile in the Atlμs menu. See "Displaying the current profile or a saved profile" in the "Displaying Map Data" chapter for details.

Using the tool palette

The tool palette in the Profile Setup window contains tools for manipulating the displayed spectrum and specifying peak information for creating profiles (see "Creating a profile" for details). The next sections explain how to use the tools.

Note The annotation tool is not used for creating a profile. ▲

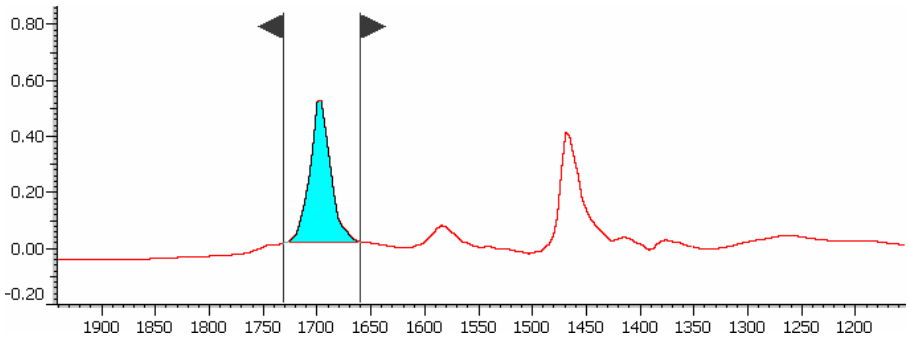
Zooming in on a portion of a spectrum

You can enlarge a portion of the displayed spectrum just as you would in a spectral window. Simply use the selection tool to draw a box around the area and then click inside the box.

Selecting a spectral region

Use the region tool to specify a spectral region for the profile. When you select the tool, two vertical lines with triangular handles appear in the spectral display pane. Drag the lines to the desired starting and ending limits of the region. The area defined by the spectrum, the two lines and the baseline is shaded: Blue shading indicates positive area (above the baseline). Gray shading indicates negative area (below the baseline). The total area is the sum of all the positive and negative areas.

Here is an example of a selected region:



If Profile Type is set to a type that uses a spectral region and baseline, the specified values appear in the appropriate text boxes.

Finding the X and Y values of a data point

You can use the spectral cursor tool to find the exact X and Y values of a data point in the displayed spectrum. Simple select the tool and then click the point. The values appear above the tool palette. Here is an example:

Specifying peak locations and baselines

When you create a new profile using the Peak Height Of One Peak or Peak Height Ratio Of Two Peaks options, you can use the peak height tool to specify the peak or peaks graphically.

Specifying a single peak

Follow these steps to specify a single peak for the Peak Height Of One Peak option (for creating a profile):

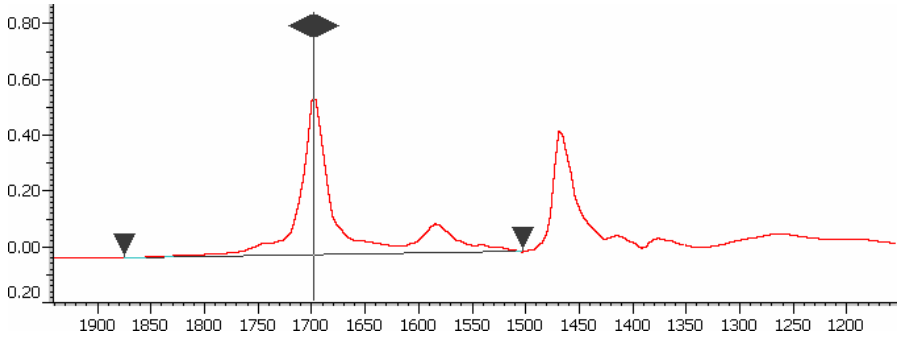
1. **Set Profile Type to Peak Height Of One Peak.**

2. **Select the peak height tool.**

   A vertical line with a diamond-shaped handle appears in the spectral display pane. A baseline also appears with two triangular handles indicating the current baseline endpoints. See the illustration in the next step.

3. **Drag the line to the desired peak location, and adjust the baseline by dragging the endpoints to new frequency locations.**

   Here is an example:



   The specified values appear in the appropriate text boxes.

Specifying two peaks

Follow these steps to specify two peaks for the Peak Height Ratio Of Two Peaks option (for creating a profile):

1. **Set Profile Type to Peak Height Ratio Of Two Peaks.**

2. **Select the peak height tool.**

   A vertical line with a diamond-shaped handle appears in the spectral display pane. A baseline also appears with two triangular handles indicating the current baseline endpoints. See the illustration in the preceding procedure.

3. **Drag the line to the desired numerator peak location, and adjust the baseline by dragging the endpoints to new frequency locations.**

   The specified values appear in appropriate the Ratio Numerator text boxes.

4. **Click one of the Ratio Denominator text boxes.**

5. **Drag the line to the desired denominator peak location, and adjust the baseline by dragging the endpoints to new frequency locations.**

   The specified values appear in the appropriate Ratio Denominator text boxes.

Specifying peak areas and baselines

When you create a new profile using the Chemigram, Peak Area Of One Peak or Peak Area Ratio Of Two Peaks options, you can use the peak area tool to specify the peak or peaks graphically. (You can also use the region tool; see "Selecting a spectral region" for details.)

Specifying a single peak area

Follow these steps to specify the area of a single peak for the Peak Area Of One Peak option or to specify a spectral region for the Chemigram option (for creating a profile):

1. **Set Profile Type to Chemigram or Peak Area Of One Peak.**

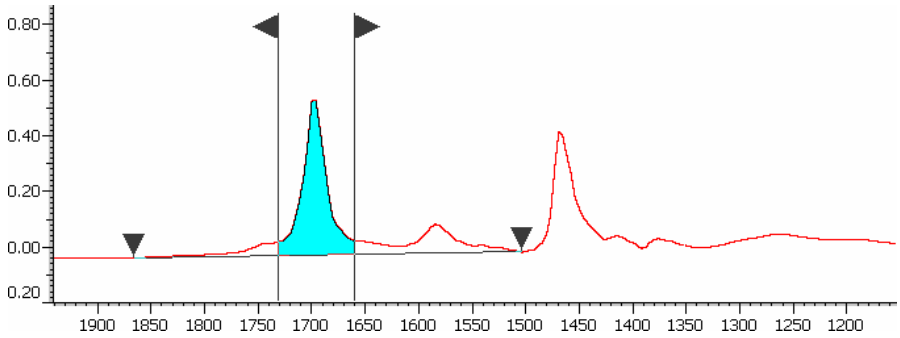
2. **Select the peak area tool.**

   Two vertical lines with triangular handles appear in the spectral display pane. A baseline also appears with two triangular handles indicating the current baseline endpoints. See the illustration in the next step.

3. **Drag the lines to the starting and ending limits of the desired spectral region, and adjust the baseline by dragging the endpoints to new frequency locations.**

   The area defined by the spectrum, the two lines and the baseline is shaded: The area defined by the spectrum, the two lines and the baseline is shaded: Blue shading indicates positive area (above the baseline). Gray shading indicates negative area (below the baseline). The total area is the sum of all the positive and negative areas.

Here is an example of a specified area:



The specified values appear in the appropriate text boxes.

Specifying two peak areas

Follow these steps to specify the areas of two peaks for the Peak Area Ratio Of Two Peaks option (for creating a profile):

1. **Set Profile Type to Peak Area Ratio Of Two Peaks.**

2. **Select the peak area tool.**

   Two vertical lines with triangular handles appear in the spectral display pane. A baseline also appears with two triangular handles indicating the current baseline endpoints. See the illustration in the preceding procedure.

3. **Drag the lines to the desired starting and ending limits of the numerator spectral region, and adjust the baseline by dragging the endpoints to new frequency locations.**

   The area defined by the spectrum, the two lines and the baseline is shaded: The area defined by the spectrum, the two lines and the baseline is shaded: Blue shading indicates positive area (above the baseline). Gray shading indicates negative area (below the baseline). The total area is the sum of all the positive and negative areas.

   The specified values appear in the appropriate Ratio Numerator text boxes.

4. **Click one of the Ratio Denominator text boxes.**

5. **Drag the lines to the desired starting and ending limits of the denominator spectral region, and adjust the baseline by dragging the endpoints to new frequency locations.**

   The specified values appear in the appropriate Ratio Denominator text boxes.

Converting a map to other units

You can use the Process menu commands listed below to convert the spectra in an infrared map to different Y-axis units.

Use this command…	To convert to these units…
Absorbance	absorbance
% Transmittance	% transmittance
Other Conversions	Kubelka-Munk, % reflectance or log (1/R)

For more information and instructions, find "units" in the OMNIC Help system Index and go to the appropriate topic: "Converting spectra to absorbance," "Converting spectra to % transmittance" or "Converting spectra to special units" (for the Other Conversions command).

If you convert a map's units, you will be asked whether to save the map when you close it. We recommend that you convert and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

Reprocessing a map

Reprocess Map in the Atlμs menu lets you transform the interferogram data for an infrared map using different transform parameter settings or ratio the map spectra against a different background in order to improve the final data. You can use any stored background spectrum and change the settings several parameters. Only maps collected with the interferograms saved can be reprocessed. See "Saving interferograms with the map" in the "Preparing for Data Collection" chapter for more information.

Follow these steps to reprocess the active infrared map:

1. **Choose Reprocess from the Process menu.**

   The Reprocess dialog box appears showing the current settings of the transform parameters.

2. **If you want to change the setting of a parameter, select a setting from the drop-down list box to the right of the parameter name.**

   You can select a resolution that is less than or equal to that of the original map.

3. **If you want to reprocess the map using a different background, use the Browse button to locate and select a background.**

4. **When the parameters and background file are set the way you want them, choose OK to reprocess the map.**

Retrieving interferograms saved with map spectra

Choose Retrieve Interferograms from the Process menu to display in a spectral window the sample and background interferograms for the selected sample point of the infrared active map. (To select a point, click it in the contour map, video image or 3-D image.) To be retrieved and displayed, the interferograms must have been saved when the map spectra were collected. See "Saving interferograms with the map" in the "Preparing for Data Collection" chapter for more information.

If you discover a problem with the transformed data, you may be able to diagnose the problem by examining the interferogram.

Saving an area map profile as a CSV text file

Use Save Profile As CSV Text in the Atlμs menu to save all the profile data of an area map in a map window or profile window as a CSV (comma-separated values) text file. You can open the saved file later using an application that opens CSV files. Follow these steps:

1. **Choose Save Profile As CSV Text from the Atlμs menu.**

   The Save As dialog box appears.

2. **Type a file name in the File Name text box.**

   Use the file extension .CSV.

3. **Locate and open the directory where you want the profile saved.**

4. **Choose OK.**

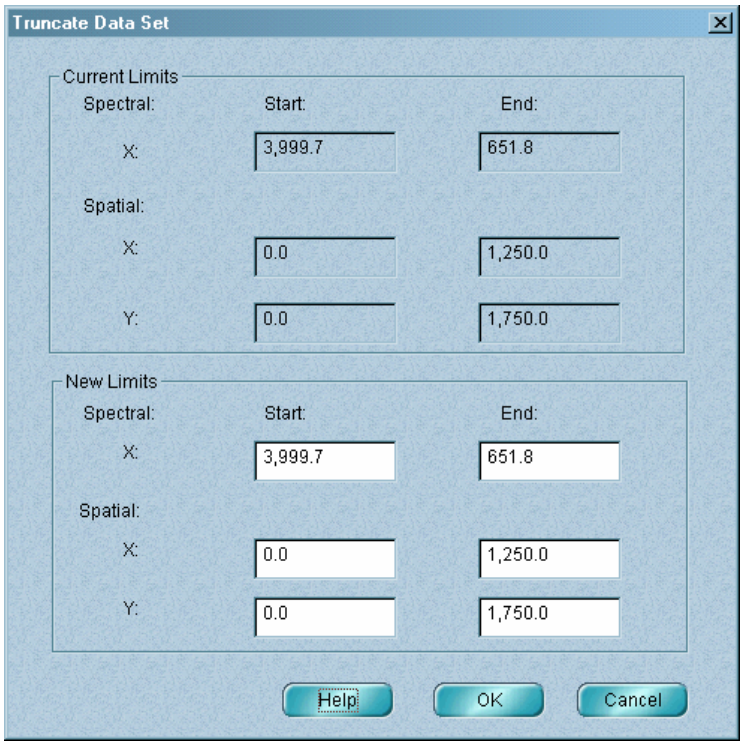
Truncating the spectral and spatial ranges of a map

Use Truncate Data Set in the Atlμs menu to permanently delete from the active map all the spectral data outside a specified spectral region and spatial area of the sample. This is useful for reducing the size of large maps and speeding up interactions with them. It is also useful for eliminating noisy data. If you think you may need the deleted data later, save the map using a different name before you truncate the spectral range.

Follow these steps:

1. **Choose Truncate Data Set from the Atlμs menu.**

   The Truncate Data Set dialog box appears. Here is an example showing the parameters for an area map:



   The Current Limits box displays the current spectral frequency limits and, below them, the current X and Y spatial limits, if applicable.

   For an area depth profile, the spatial X values indicate the horizontal distance limits (along the top edge of the mapped vertical area), and the spatial Z values indicate the vertical distance limits.

For a line map or line depth profile only one spatial dimension appears. It represents distance along the line of the map.

For an area depth profile, spatial Z limits appear instead of Y limits. They represent depth.

For a discrete point map only the spectral range can be changed.

2. **Type the desired spectral frequency limits in the Spectral text boxes in the New Limits box.**

   The spectra in the resulting map will contain data only within these limits.

3. **Type the desired spatial limits in the Spatial text boxes in the New Limits box (if available).**

   The resulting map will contain only those spectra collected at sample points within these limits.

4. **Choose OK.**

   The spectral data outside the specified regions is deleted from the map. This can take several minutes.

Tips Truncating the spectral range of a map

You can use Truncate Data Set to isolate spectral regions having relatively high signal-to-noise ratios (SNR). If the SNR is poor, it will be poorest at the low-wavenumber end of the spectral range. You can eliminate that portion of the range by truncating the map spectra. If you fail to eliminate bad data from the map, misleading profiles may result, especially if the map has been baseline-corrected.

Extracting a line map from an area map

Use Extract Line Map in the Atlμs menu to create a new line map from spectra contained in the active area map. The new map is displayed in a new map window. Follow these steps:

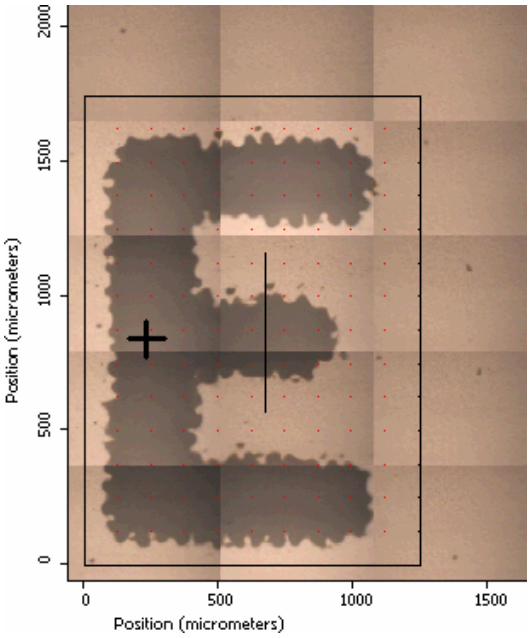
Note If you prefer to specify the line numerically, skip to step 2. ▲

1. **Use the mouse to draw the desired line across the area contour map or the video image.**

   If a line map icon (shown below) appears next to the pointer when it is in the contour map pane or video pane, you can draw the line in either pane.

   If the line map icon is absent, first *right-click* anywhere in the contour map pane or video pane, point to Cursor Mode in the pop-up menu and then choose Extract Line Map. You can then draw a line in either pane.

   Here is an example showing a line drawn in the video pane:

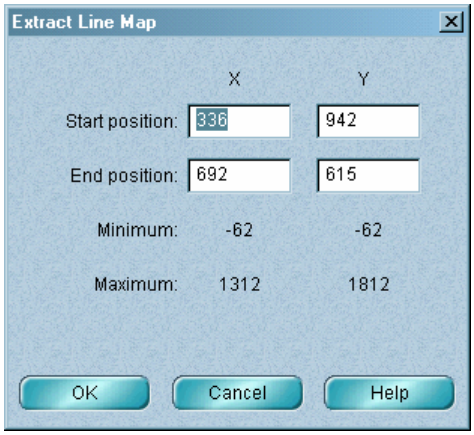


You can move the line or change its length or slope: Simply point to the line's center or an endpoint so that directional arrows appear, and then drag the line or the endpoint to the desired location.

2. **Choose Extract Line Map from the Atlμs menu.**

   The Extract Line Map dialog box appears:

If you drew a line in step 1, the X and Y values of its endpoints appear in the dialog box.



   The minimum and maximum X and Y values of the map data appear below the text boxes. The X and Y values of the start and end of the line must be within this range of values.

3. **Type the X and Y values you want used for the line endpoints in the appropriate text boxes, or make any desired changes to the displayed values.**

4. **Choose OK.**

   The line map is calculated and displayed in a new map window.

Viewing, editing or creating functional groups

Use Edit Functional Groups in the Atlμs menu to view, edit or delete existing user-defined functional groups or create new functional groups to be used for creating profiles. A functional group in OMNIC Atlμs shows the locations of a chemical functional group on a sample.

When you specify the spectral regions for a functional group, you also specify a weighting factor for each region. The weighting factor determines the degree to which a region influences spectral differentiation. Using a weighting factor for each region is necessary, since many functional groups have more than one band that can be used to confirm the group's presence in a sample. Assign a larger weighting factor to regions that are more helpful in differentiating the group from other groups.

After you create a functional group, it becomes available for your selection when you set up a profile with Profile Setup in the Atlμs menu. See "Creating a profile" in the "Processing and Analyzing Map Data" chapter for details on creating profiles.

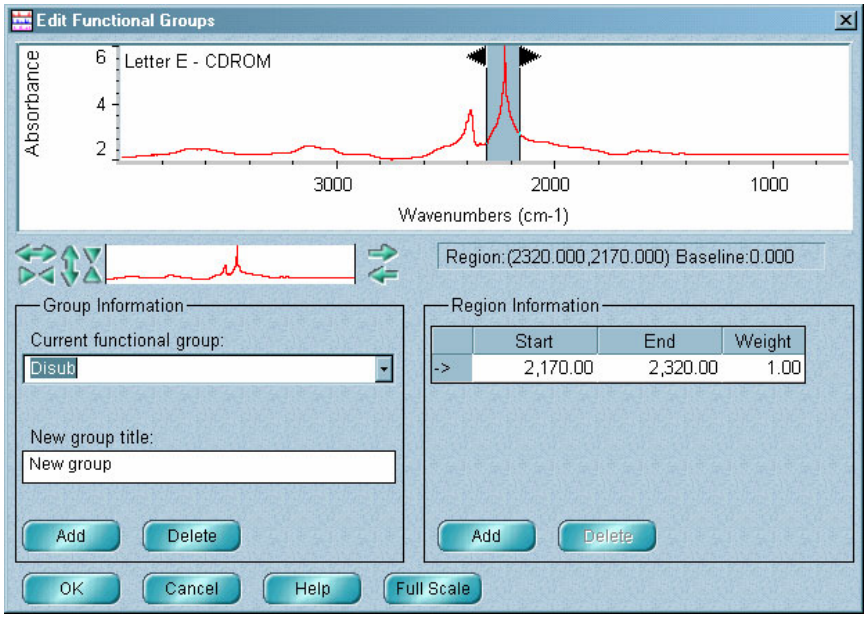
Follow these steps to view, edit or create functional groups:

1. **In the map window, display a spectrum of a compound that contains one or more functional groups of interest.**

   Displaying a spectrum that contains bands caused by the functional groups can help you specify the spectral regions for the groups graphically. (You will also be able to specify the regions by typing their numerical region limits.)

2. **Choose Edit Functional Groups from the Atlμs menu.**

   The Edit Functional Groups window appears with the spectrum in the pane near the top of the window. Here is an example:



   The Region Information box contains a table showing the frequency limits of the spectral regions currently specified for the functional group indicated by the Current Functional Group drop-down list box. If you click a row of the table, the spectral region specified by that row is indicated in the pane by a shaded area between two vertical region markers. An arrow near the left edge of the table shows which spectral region is currently indicated in the pane. When needed, a scroll bar is provided for scrolling rows of the table into view.

   Each spectral region has a weighting factor, shown in the Weight column of the table.

3. **To view the region information for a particular functional group, select the group from the Current Functional Group drop-down list box.**

4. **If desired, edit the region information for the current functional group.**

   To do this, click the row of the table that specifies the spectral region you want to change and then drag the handles of the region markers in the pane to the desired frequency limits. The X values of the marker locations appear in the readout below the pane to help you position the markers precisely.

   You can also specify a region limit by double-clicking the current limit in the table, typing a new value and then pressing Enter.

   You can change the view of the spectrum to see a region more clearly by using the view finder below the pane. (See the OMNIC Help system if you need information on using the view finder.) If you want to display the spectrum "full scale" so that it fills the pane vertically, click the Full Scale button at the bottom of the window.

   If you want to change the weighting factor for a region, double-click the factor in the table, type a new value and then press Enter.

   You can add a spectral region to the table by clicking the Add button in the Region Information box. A row is added to the bottom of the table. Edit the region limits and weighting factor in the row as described above.

   You can delete an entire spectral region specification by clicking its row in the table and then clicking the Delete button in the Region Information box.

5. **If desired, create one or more new functional groups.**

   To create a group, type a title for the group in the New Group Title box and then click the Add button in the Group Information box. The new title appears in the Current Functional Group drop-down list box.

   Specify the spectral regions for the group and their weighting factors by using the editing methods described above.

You can delete an entire functional group specification by selecting the group from the Current Functional Group drop-down list box and then clicking the Delete button in the Group Information box.

6. **If desired, change the title of one or more functional groups.**

   To edit a title, first select the group whose title you want to change from the Current Functional Group drop-down list box. The title text is automatically selected and ready to change. Type a new title or use standard techniques to edit the title text.

7. **When you are finished viewing or specifying the functional groups and their spectral regions, choose OK.**

Correcting map spectra

OMNIC Atlμs provides features for correcting map spectra in the following ways:

- Remove dispersion effects.
- Remove the effects of water absorptions.
- Remove the effects of carbon dioxide absorptions.
- Automatically correct the baselines of all the spectra in a map.
- Correct attenuated total reflection (ATR) spectra for the shifting of infrared absorption bands and the effects of variation in depth of penetration.

The next sections explain how to use the features.

Correcting the baselines of map spectra automatically

Use Automatic Baseline Correct in the Process menu to automatically correct the tilted baselines of map spectra, with the baseline points selected by the software. In OMNIC Help Topics find "baseline" in the Index and go to "Correcting baselines automatically" for more information and instructions.

If you correct a map, you will be asked whether to save the map when you close it. We recommend that you correct and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

Using Advanced ATR Correction

Use Advanced ATR Correction in the Process menu to correct attenuated total reflection (ATR) spectra in the active map for the shifting of infrared absorption bands and the effects of variation in depth of penetration. In OMNIC Help Topics find "ATR correction" in the Index and go to "Using Advanced ATR Correction" for more information and instructions.

If you correct a map, you will be asked whether to save the map when you close it. We recommend that you correct and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

Correcting map spectra for dispersion effects or water and carbon dioxide absorptions

Use Other Corrections in the Process menu to correct map spectra for dispersion effects (select the Kramers-Kronig option) or water or carbon dioxide absorptions. In OMNIC Help Topics find "Other Corrections command" in the Index and go to "Using Other Corrections" for more information and instructions.

If you correct a map, you will be asked whether to save the map when you close it. We recommend that you correct and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

Blanking a spectral region

Use Blank in the Process menu to delete the data points in the specified spectral region of your map spectra. This is useful, for example, when the spectra contain totally absorbing peaks that would cause poor library search results. In OMNIC Help Topics find "Blank command" in the Index and go to "Blanking a spectral region" for more information about the uses of Blank.

If you blank a spectral region of a map, you will be asked whether to save the map when you close it. We recommend that you blank the region and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

You can specify the spectral region graphically or numerically, as explained in the following procedures.

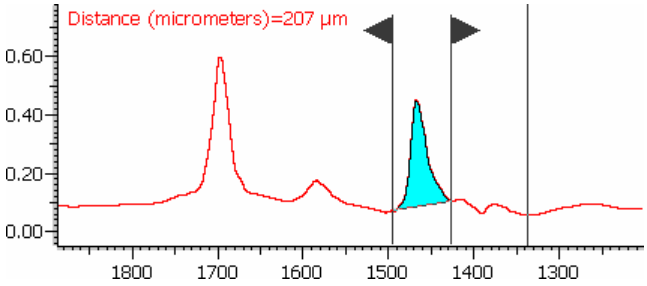
Follow these steps if you want to specify the spectral region graphically:

1. **Set the spectral display pane cursor to region mode if it is in zoom mode.**

   The cursor is in zoom mode if no vertical lines with triangular handles appear in the pane. To set the cursor to region mode, *right-click* anywhere in the pane, point to Cursor Mode in the pop-up menu and then choose Region. Two vertical lines appear (see the illustration in the next step).

2. **Drag the lines by their triangular handles to the desired starting and ending frequencies.**

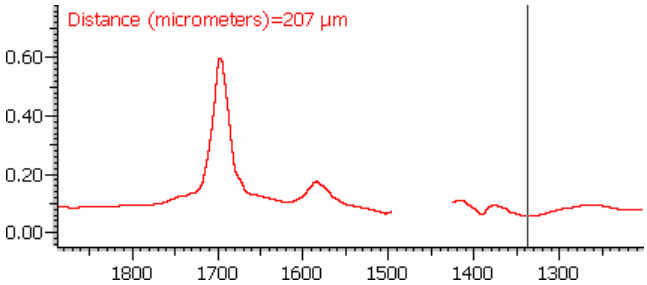
   Here is an example:



   The peak area between the two lines is shaded. The data points in this region will be deleted.

3. **Choose Blank from the Process menu.**

   The data points in the region are deleted:



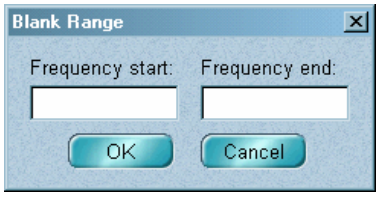
Follow these steps if you want to specify the spectral region numerically:

1. **Set the spectral display pane cursor to zoom mode if it is in region mode.**

   The cursor is in region mode if two vertical lines with triangular handles appear in the pane. To set the cursor to zoom mode, *right-click* anywhere in the pane, point to Cursor Mode in the pop-up menu and then choose Zoom.

2. **Choose Blank from the Process menu.**

   The Blank Range dialog box appears:



3. **Type the X-axis limits of the region to blank in the Frequency Start and Frequency End text boxes.**

4. **Choose OK.**

   The data points in the region are deleted. See the example at the end of the preceding procedure.

Replacing a spectral region with a straight line

Straight Line in the Process menu lets you replace the selected region of your map spectra (or the displayed region if no region is selected) with data points that form a straight line. Use Straight Line to remove unwanted spectral features in order to improve the appearance of spectra. In OMNIC Help Topics find "Straight Line command" in the Index and go to "Replacing a spectral region with a straight line" for more information.

If you replace a spectral region of a map, you will be asked whether to save the map when you close it. We recommend that you replace the region and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

You can specify the spectral region graphically or numerically, as explained in the following procedures.

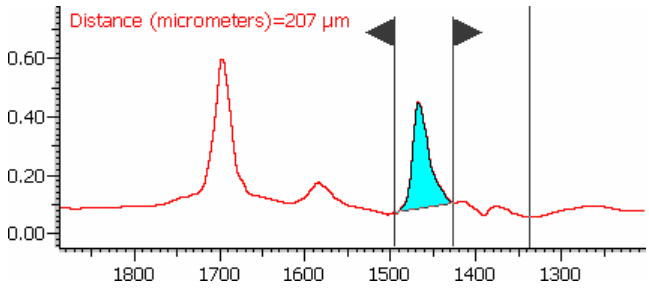
Follow these steps if you want to specify the spectral region graphically:

1. **Set the spectral display pane cursor to region mode if it is in zoom mode.**

   The cursor is in zoom mode if no vertical lines with triangular handles appear in the pane. To set the cursor to region mode, *right-click* anywhere in the pane, point to Cursor Mode in the pop-up menu and then choose Region. Two vertical lines appear (see the illustration in the next step).

2. **Drag the lines by their triangular handles to the desired starting and ending frequencies.**

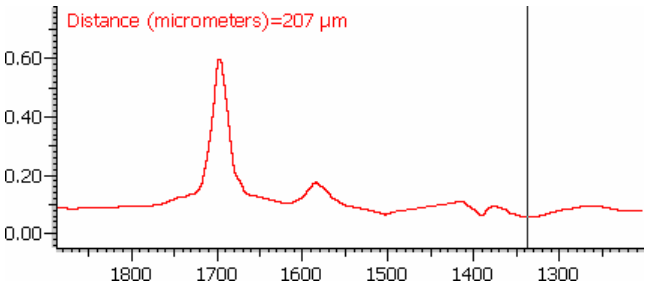
   Here is an example:



The peak area between the two lines is shaded, and a baseline shows where the straight line will appear when the region is replaced.

3. **Choose Straight Line from the Process menu.**

   The region is replaced with a straight line:



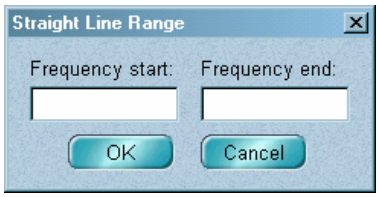
Follow these steps if you want to specify the spectral region numerically:

1. **Set the spectral display pane cursor to zoom mode if it is in region mode.**

   The cursor is in region mode if two vertical lines with triangular handles appear in the pane. To set the cursor to zoom mode, *right-click* anywhere in the pane, point to Cursor Mode in the pop-up menu and then choose Zoom.

2. **Choose Straight Line from the Process menu.**

   The Straight Line Range dialog box appears:



3. **Type the X-axis limits of the region you want to replace in the Frequency Start and Frequency End text boxes.**

4. **Choose OK.**

   The region is replaced with a straight line. See the example at the end of the preceding procedure.

Smoothing map data

The following sections discuss using Smooth, Automatic Smooth or Pixel Addition in the Process menu to smooth your map data.

If you smooth a map, you will be asked whether to save the map when you close it. We recommend that you smooth the map and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

Smoothing map spectra by specifying the number of smoothing points

Use Smooth in the Process menu to improve the appearance of map spectra by preferentially smoothing the high-frequency component of the spectral data. Smoothing is useful for improving the appearance of peaks obscured by noise.

Note To smooth spectra manually by specifying the degree of smoothing (setting the number of points), use Smooth. To smooth spectra automatically, use Automatic Smooth as explained in the next section. An automatic smooth often gives a satisfactory result and is faster than a manual smooth. ▲

The degree to which a spectrum is smoothed depends on the number of smooth points used and the selected polynomial order. These are explained in the following procedure.

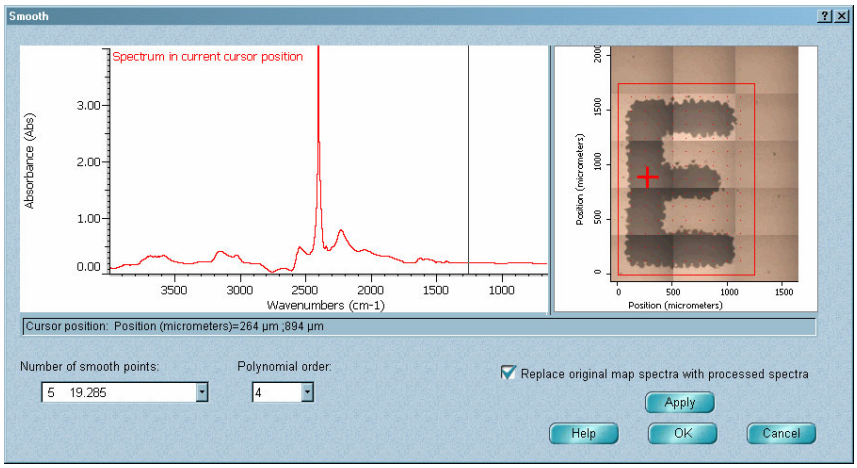
Important The smoothing algorithm smoothes all sharp peaks, including sample peaks. Be careful when smoothing spectra with real sample peaks that are narrow, since these features will also be smoothed. ▲

Note Smoothing degrades the effective spectral resolution of the data and can remove ("smooth out") small spectral features. An alternative to smoothing is to collect more scans. ▲

Follow these steps to smooth the spectra in the active map:

1. **Choose Smooth from the Process menu.**

   The Smooth window appears:



   The spectral display pane contains the spectrum collected at a point indicated by the cross hairs in the video image. Except for the case of a line depth profile, you can display a different spectrum by clicking another point in the video image or dragging the cross hairs. The location of the point appears below the spectral display pane.

2. **Specify whether to replace the original map spectra.**

   If you select Replace Original Map Spectra With Processed Spectra (the default), the original spectra will be replaced by the smoothed spectra when you choose OK. If this option is not selected, the original map will appear in the map window and both the original and smoothed spectra will be saved in the map file. When you open the map later, you will be asked whether to display the original or processed spectra.

3. **Specify the desired number of smooth points by setting Number Of Smooth Points.**

   The value to the right of the number of points represents the frequency range that is considered when smoothing a point in a spectrum. The value is the product of the number of smooth points and the data spacing.

   You can set the number of points to any odd number from 5 to 25. A larger number of points results in a greater degree of smoothing. You should normally smooth using the minimum number of points that produce the desired result.

   For moderate smoothing of a spectrum at 4- or 8-wavenumber resolution, start with 5, 7 or 9 points. Compare the sharpest bands in the original spectra with the same bands in the smoothed spectra to determine whether the resolution was degraded significantly. If the resolution was not significantly degraded, increase the number of points and smooth again if needed. Otherwise, decrease the number of points and smooth again.

4. **Specify the desired polynomial order by setting Polynomial Order.**

   You can set the polynomial order to any number from 1 to 6. A higher order results in less smoothing; lower orders cause more smoothing. Typically a setting of 3 (for cubic polynomial) is used for average smoothing.

Note The setting of Polynomial Order must be smaller than the setting of Points. If the polynomial order is greater than the number of data points for smoothing, any additional polynomial coefficients are automatically set to zero. ▲

5. **To see the effects of your settings, choose Apply.**

   The smoothed spectrum is overlaid on the original spectrum. You can change the settings and choose Apply again to see the effect of the new settings.

6. **When you are finished, choose OK.**

Smoothing map spectra automatically

Use Automatic Smooth in the Process menu to improve the appearance of map spectra by preferentially smoothing the high-frequency component of the spectral data. Smoothing is useful for improving the appearance of peaks obscured by noise. In OMNIC Help Topics find "Automatic Smooth command" in the Index and go to "Smoothing spectra automatically" for more information and instructions.

If you want to specify the number of smoothing points, use Smooth in the Process menu. See the preceding section for details.

Changing the data spacing

Use Change Data Spacing in the Process menu to change the spatial and spectral spacing of the active map. (For a discrete point map only the spectral data spacing can be changed.) Spatial data spacing is distance between adjacent sample points on the sample surface. Spectral data spacing is the number of wavenumbers between data points in a spectrum. It is determined by the resolution and zero filling settings used when you collect the data.

If you use this command to change the spectral data spacing to a higher value, the software deresolves the data. If you change the spectral data spacing to a lower value, the software zero fills the data; that is, it adds interpolated data points between the existing data points.

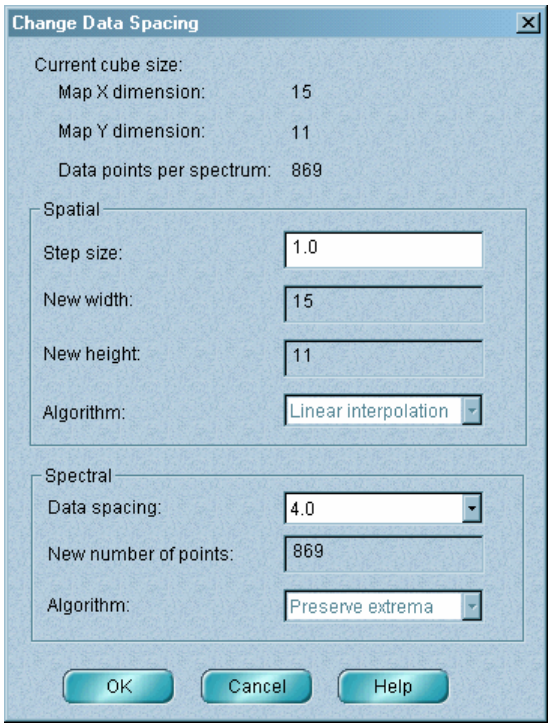
You can best compare two maps if they have the same spectral data spacing. If the maps were collected using different spacings, you can use this command to change the spacing of one to match the other.

In quantitative analysis the spectral data spacing must match that of the standard spectra used to develop the method. Use this command when necessary to change the spectral data spacing of the map to match the standards before creating a profile showing quantitative analysis results.

Follow these steps to change the data spacing of a map:

1. **Choose Change Data Spacing from the Process menu.**

   The Change Data Spacing dialog box appears. Here is an example:



For a discrete point map only the spectral data spacing can be changed.

   The current dimensions (in steps) of the map and the number of data points per spectrum appear at the top of the dialog box.

2. **Change the spatial data spacing if desired.**

   Skip to step 3 if you are displaying a discrete point map.

   The current step size (the distance between points) is considered to be 1. Changes you make to the step size will be relative to this value.

   For a line map or line depth profile the New Width value shows the number of steps in the line; the New Height value does not apply.

For an area map the New Width value shows the number of steps along the width of the map, and the New Height value shows the number of steps along the height of the map. For an area depth profile the New Width value shows the number of horizontal steps, and the New Height value shows the number of vertical (Z dimension) steps.

- **To increase the step size**, and thus remove existing sample points from the map to spatially deresolve the data, type a value greater than 1 in the Step Size text box. The New Width and New Height values, if applicable, automatically decrease to reflect the change.

  Then specify the algorithm for the operation by setting Algorithm. The Preserve Extrema setting tends to preserve the full amplitude of peaks. The Average setting averages all the data equally, resulting in smaller peaks.

- **To decrease the step size**, and thus add interpolated sample points between existing points in the map, type a value less than 1 in the Step Size text box. The New Width and New Height values, if applicable, automatically increase to reflect the change.

  Then specify the interpolation to use for adding sample points by selecting an algorithm from the Algorithm drop-down list box. The Linear Interpolation setting calculates the intensity values of the new points in a simple, linear manner. The Spline Interpolation setting uses a cubic polynomial to calculate values.

3. **Change the spectral data spacing if desired.**

   The current data spacing appears in the Data Spacing drop-down list box.

   - **To increase the data spacing**, and thus remove existing data points from the spectra to deresolve the data, set Data Spacing to a greater value. The New Number Of Points value automatically decreases to reflect the change.

     Then specify the algorithm for the operation by setting Algorithm. The Preserve Extrema setting tends to preserve the full amplitude of peaks. The Average setting averages all the data equally, resulting in smaller peaks.

- **To decrease the data spacing**, and thus add interpolated data points between existing points in the spectra, set Data Spacing to a smaller value. The New Number Of Points value automatically increases to reflect the change.

  Then specify the interpolation to use for adding data points by selecting an algorithm from the Algorithm drop-down list box. The Linear Interpolation setting calculates the intensity values of the new points in a simple, linear manner. The Spline Interpolation setting uses a cubic polynomial to calculate values.

4. **Choose OK.**

Performing math operations on map spectra

OMNIC Atlμs provides several commands in the Process menu for performing math operations on map spectra. The next sections explain how to use these commands.

Performing a scaled subtraction on map spectra

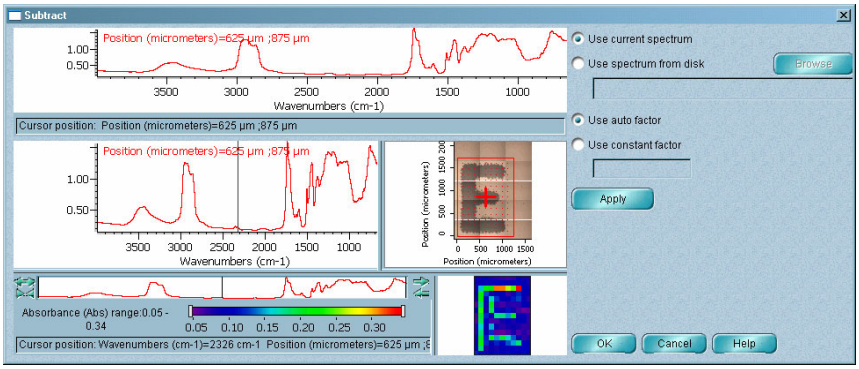
Use Subtract in the Process menu to subtract a spectrum from the spectra of the active map.

If you perform a subtraction on a map, you will be asked whether to save the map when you close it. We recommend that you perform the subtraction and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

Follow these steps to perform a scaled subtraction:

1. **Choose Subtract from the Process menu.**

   The Subtract window appears:



   The upper spectral display pane contains the spectrum collected at a point indicated by the cross hairs in the video image. Except for the case of a line depth profile, you can display a different spectrum by clicking another point in the video image or dragging the cross hairs. The location of the point appears below the color bar.

   The lower spectral display pane is used to display the result spectrum.

2. **Specify the spectrum to subtract.**

   - To subtract the spectrum displayed in the upper spectral display pane, select Use Current Spectrum. You can display a different spectrum by clicking another location in the video image.

     You can use the sky view control just as you would in a map window to adjust the display of the video image. See "Adjusting the display with the sky view control" in the "Displaying Map Data" chapter for details.

   - To subtract another spectrum stored on a disk, select Use Spectrum From Disk. Then type the pathname of the desired spectrum in the text box, or use the Browse button to locate and select a spectrum.

3. **Specify the subtraction factor.**

   The specified spectrum will be multiplied by a subtraction factor before being subtracted from the map spectra. This lets you compensate for unequal spectral intensities in the specified spectrum and the map spectra, giving better subtraction results.

   - To use a subtraction factor that is calculated automatically, select Use Auto Factor.

   - To use a constant factor that you specify, select Use Constant Factor and then type the desired factor in the Constant text box.

4. **To see the subtraction result, choose Apply.**

   You can change your settings and choose Apply again to see the effect of the new settings.

5. **When you are satisfied with the subtraction result, choose OK.**

Subtracting a component or contaminant from map spectra

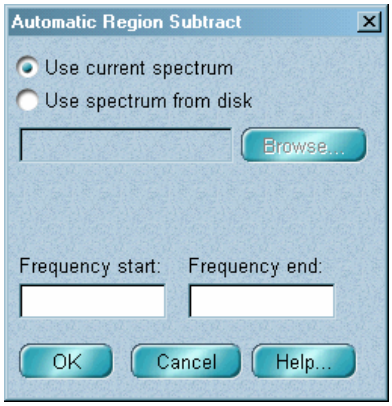
Use Automatic Region Subtract command in the Process menu to subtract from the spectra of the active map the spectral data due to a particular component or contaminant. By selecting the region of a reference spectrum that contains the undesirable peaks, you allow the software to automatically determine the subtraction factor that will best eliminate those peaks. In OMNIC Help Topics find "component" in the Index and go to "Subtracting a component or contaminant from a mixture spectrum" for more information.

If you perform a subtraction on a map, you will be asked whether to save the map when you close it. We recommend that you perform the subtraction and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

Follow these steps to subtract a component or contaminant from a map:

1. **Choose Automatic Region Subtract from the Process menu.**

   The Automatic Region Subtract dialog box appears:



2. **Specify the reference spectrum that contains the component peaks.**

   - To use the spectrum displayed in the spectral display pane of the map window, select Use Current Spectrum.

   - To use another spectrum stored on a disk, select Use Spectrum From Disk. Then type the pathname of the desired spectrum in the text box, or use the Browse button to locate and select a spectrum.

3. **Enter the X-axis limits of the region that contains the component peaks in the Frequency Start and Frequency End text boxes.**

   The software uses this region to automatically determine the subtraction factor.

4. **Choose OK.**

Multiplying map spectra by a number

Use Multiply in the Process menu to multiply each data point in a your map spectra by a number of your choice. This is useful when you want to scale the spectra so that data of very different intensities can be compared. By making the intensity of a peak in one spectrum match that of the same peak in another spectrum, you can see how the relative intensities of the other peaks compare. In OMNIC Help Topics find "Multiply command" in the Index and go to "Multiplying a spectrum by a number" for more information and instructions.

If you multiply a map by a number, you will be asked whether to save the map when you close it. We recommend that you perform the multiplication and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

Converting map spectra to their first and second derivatives

Use Derivative in the Process menu to convert the spectra in the active map to their first or second derivatives.

The first derivative is useful for revealing peaks that appear as shoulders in the original spectra. It shows the rate of change across the entire spectrum. This means that in the first derivative, shoulders become narrower and thus are easier to see. It is important to remember that the maximum and minimum points in the first derivative curve are the points of maximum rate of change and not the maximum and minimum points of the original peaks. The maximum and minimum points of the original peaks have a Y value of zero in the first derivative.

Use the second derivative to find the exact location (center) of shoulders in the original spectra. It shows the change in the rate of change across the spectrum. This curve is more complex than the first derivative, with significantly narrower bands. The second derivative is useful for finding exact peak locations since peaks in the second derivative appear at the same locations as peaks in the original spectrum. The second derivative has more baseline noise than the first derivative. For each derivative operation you perform, the noise level increases slightly, the signal strength decreases dramatically and the signal-to-noise ratio decreases.

You can specify that the conversion be done using no filter, using the Savitzky-Golay derivative filter, or using the Norris derivative filter:

- Select the First Difference Derivative option if you do not want to use a filter.

- The Savitsky-Golay Derivative option is useful for improving the appearance of peaks that are obscured by noise. It uses the specified number of data points and polynomial order to determine the degree of smoothing for the conversion.

  You can set the number of data points to any odd number from 3 to 51. A larger number results in a greater degree of smoothing. You should normally smooth using the minimum number of data points that produce the desired result. Typically a setting of 7 is used for average smoothing.

  For moderate smoothing of a spectrum at 4- or 8-wavenumber resolution, start with a setting of 5, 7 or 9. Compare the sharpest bands in the original spectrum with the same bands in the smoothed spectrum to determine whether the resolution was degraded significantly. If it was not, increase the number of data points and smooth again if needed.

  You can set the polynomial order to any number from 1 to 6 (the default value is 3). A higher polynomial order results in less smoothing; lower orders cause more smoothing. Typically a setting of 3 (for cubic polynomial) is used for average smoothing.

Note The setting of Polynomial Order must be smaller than the setting of Points. If the polynomial order is greater than the number of data points for smoothing, any additional polynomial coefficients are automatically set to zero. ▲

Important The Savitzky-Golay algorithm smoothes all peaks. Smoothing degrades the effective spectral resolution of the data and can remove ("smooth out") small spectral features, including sample peaks, especially those in mid-IR spectra. ▲

- The Norris Derivative option is typically applied to near-IR spectra. It is often used to enhance a sharp band that is overlapped by another broad band. It is also useful for improving the appearance of peaks that are obscured by noise.

  The Norris Derivative option uses the segment length and gap between segments to determine the degree of smoothing. We define the gap between segments as the distance, in number of data points, between two consecutive segments.

  You can set the segment length to any odd number from 1 to 51 (the default value is 5). Increasing the length results in greater smoothing, since the length determines how many points are averaged.

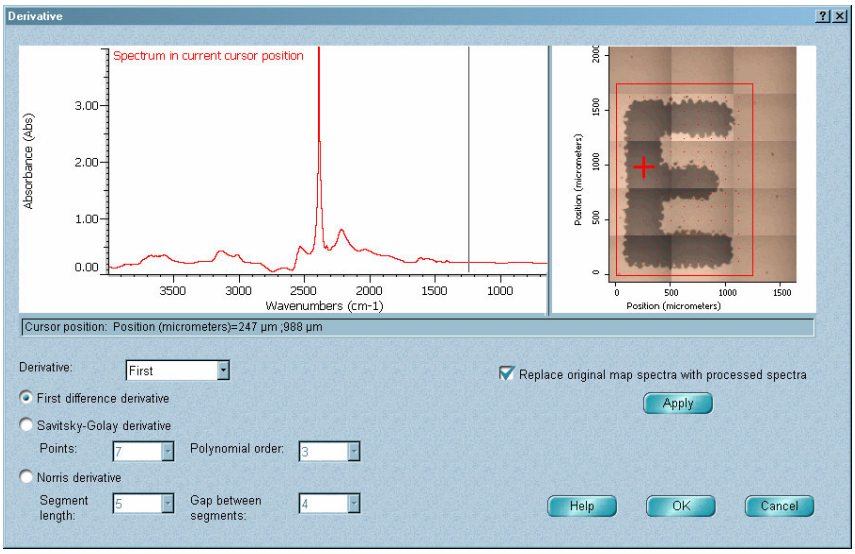
  You can set the size of the gap to any number from 1 to 20 (the default value is 5). Increasing the gap may enhance a sharp band that is overlapped by another broad band. A larger gap will also produce larger differences for broad peaks and tend to lower the resolution of the spectrum.

If you convert a map, you will be asked whether to save the map when you close it. We recommend that you convert the map and then save a copy of the map using a different file name (with Save Map As in the File menu), unless you are sure that you want to change the original data permanently.

Follow these steps to convert map spectra to their derivatives:

1. **Choose Derivative from the Process menu.**

   The Derivative window appears:



   The spectral display pane contains the spectrum collected at a point indicated by the cross hairs in the video image. Except for the case of a line depth profile, you can display a different spectrum by clicking another point in the video image or dragging the cross hairs. The location of the point appears below the spectral display pane.

2. **Specify whether to replace the original map spectra.**

   If you select Replace Original Map Spectra With Processed Spectra (the default), the original spectra will be replaced by the derivative spectra when you choose OK. If this option is not selected, the original map will appear in the map window and both the original and derivative spectra will be saved in the map file. When you open the map later, you will be asked whether to display the original or processed spectra.

3. **Select a derivative order from the drop-down list box.**

4. **Select the filter option to use.**

   If you selected First Difference Derivative, go to step 6. If you selected another option, continue with the next step.

5. **Set the parameters for the selected filter option.**

   - If you selected Savitsky-Golay Derivative, set Points to an odd number from 3 to 51; a higher setting results in greater smoothing. Set Polynomial Order to any number from 1 to 6; a higher setting results in less smoothing.

   - If you selected Norris Derivative, set Segment Length to an odd number from 1 to 51; a higher setting results in greater smoothing. Set Gap Between Segments to any number from 1 to 20; a higher value tends to lower the resolution of the spectrum.

6. **To see the effect of your settings, choose Apply.**

   The derivative spectrum is overlaid with the original spectrum. You can change the settings and choose Apply again to see the effect of the new settings.

7. **When you are finished, choose OK.**

Performing spectral math operations

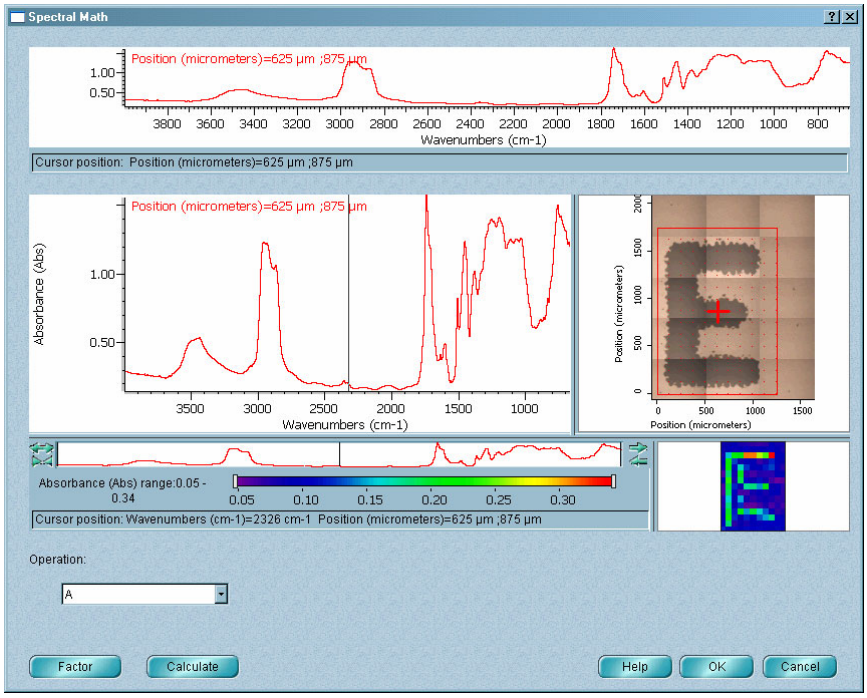
Use Spectral Math in the Process menu to perform spectral math operations on spectra in the active map. When you choose the command, the Spectral Math window appears letting you select one of the operations described in the following table.

Operation	Description
A	The original spectrum is unchanged.
A + k	The factor k is added to the Y value of each data point. Use the Factor button as explained in the following procedure to specify k.
-log(A)	The software calculates the negative logarithm of the Y value of each data point. This is the inverse of the exp(-A) operation.
exp(-A)	For each data point the natural log base e is raised to the negative power of the Y value; that is, e^{-Y}. This is the inverse of the -log(A) operation.
Mean Center-Channel	The software calculates the average of the spectra in the specified spatial portion of the map and then subtracts the average from each spectrum in the map.
Mean Center-Spectrum	For each map spectrum the software calculates the average Y value for all the data points in the spectrum and then subtracts this value from the Y value of each data point. The average Y value of each resultant spectrum is zero. You can specify spectral regions to exclude before the average Y values are calculated.
Variance Scaling	For each map spectrum the software calculates the standard deviation of the Y values of all the data points in the spectrum and then divides the Y value of each data point by the standard deviation. The standard deviation of the Y values of all the data points in each resultant spectrum is one. You can specify spectral regions to exclude before the average Y values are calculated.

Follow these steps to perform spectral math operations on the spectra in the active map:

1. **Choose Spectral Math from the Process menu.**

   The Spectral Math window appears:



   The upper spectral display pane contains the spectrum collected at a point indicated by the cross hairs in the video image. Except for the case of a line depth profile, you can display a different spectrum by clicking another point in the video image or dragging the cross hairs. The location of the point appears below the color bar.

   You can use the sky view control to zoom in on an area in the video image just as you would in a map window. You can also zoom in by drawing a box around an area and clicking inside the box. If desired, drag the handles on the sides or corners of the box to adjust its size and shape before clicking inside it.

   You can zoom in on an area of the spectrum by drawing a box around the area and clicking inside the box. You can also change the displayed spectral region by using the view finder just as you would in a map window.

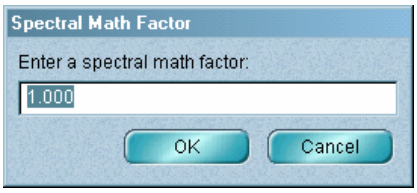
The lower spectral display pane contains the spectrum that results from the spectral math operation you perform (explained below).

You can adjust the size of the lower spectral display pane, the video image and the view finder by dragging their pane borders.

2. **Set Operation to the desired operation.**

3. **If you selected A + k, use the Factor button to specify the value of factor k.**

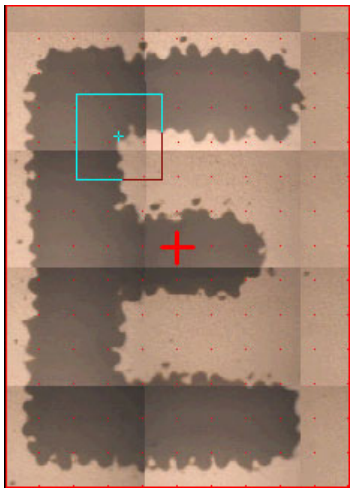
   When you choose Factor, the Spectral Math Factor dialog box appears:



   Type a new factor in the text box and then choose OK.

4. **If you selected Mean Center-Channel and want to use only a portion of the spatial area of the map for the operation, specify the portion.**

   To do this, click the video image. A box (mask) appears representing the area that will be used. Here is an example:

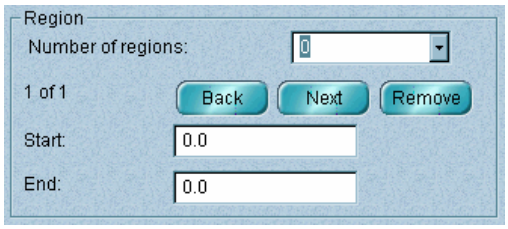


Adjust the location, size and orientation of the box so that it surrounds the desired area. To move the box, point to its center and then drag the box. To resize the box, drag any side. To rotate the box, drag any corner.

You can use the area outside the box for the operation instead of the area inside the box by selecting Invert Mask.

5. **If you selected Mean Center-Spectrum or Variance Scaling, specify the region information.**

   Use the features in the Region box:



   Specify the number of regions to exclude from the calculation by setting Number Of Regions. If you select 0, the entire spectral range of the map will be used.

   Specify the limits of the first region by typing frequency values in the Start and End text boxes or by dragging the triangular region marker handles in the lower spectral display pane. The specified region is shaded.

   To specify the next region, click the Next button and then use the techniques described above. You can click the Back button to return to the settings for the previous region. You can click the Remove button to delete a region.

6. **Choose Calculate.**

   The result spectrum appears in the lower spectral display pane.

7. **When you are satisfied with the result spectrum, choose OK.**

Normalizing the frequency of the data

Use Normalize Frequency, if available in the Process menu, to normalize the frequency of the active map. This repositions the data points at standard locations; that is, the locations they would be at if they had been collected using a system with a reference laser frequency of 15,798.0 wavenumbers.

In OMNIC Help Topics find “frequency” in the Index and go to “Normalizing the frequency of a spectrum” for more information and instructions.

Normalizing the scale of the data

Use Normalize Scale in the Process menu to change the Y-axis scale of the active map to a “normal” scale: the Y values of the data points range from 0 to 1 for the highest peak (or from 10% to 100% transmittance). This normal scale is typical of spectra in commercial spectral libraries.

In OMNIC Help Topics find “scale” in the Index and go to “Normalizing the scale of spectra” for more information and instructions.

Shifting and unshifting FT-Raman map data

You can shift and unshift FT-Raman map data by using Raman Shift, Custom Shift and Unshift in the Raman menu (if present). For instructions, in Raman Help Topics find "Raman shift" in the Index and go to "How to convert a Raman spectrum (or map) to Raman shift," "How to shift a Raman spectrum (or map) using a specified frequency" or "How to unshift a Raman spectrum (or map)."

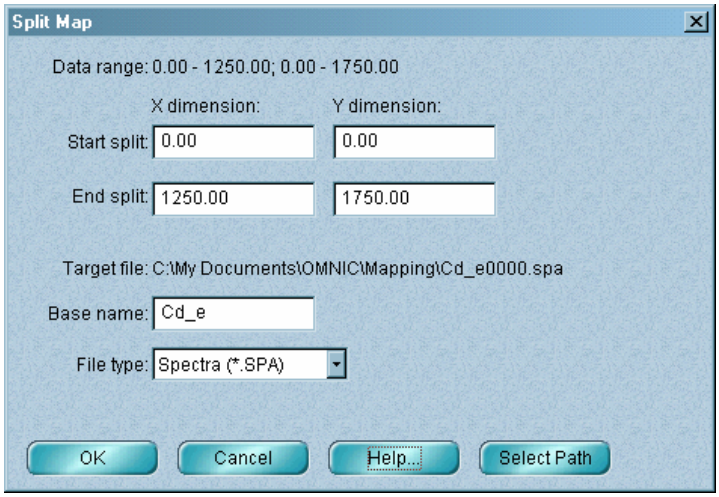
Splitting a map into separate data files

Follow the steps below to use Split Map in the Atlμs menu to split the active line map, area map, depth profile or discrete point map, or just a portion of the data, into separate .SPA, .GAML, .CSV or .JDX (JCAMP-DX) files. The new files are created by copying the specified portion of the map; the original map remains intact on the disk.

You can use Open in the File menu to open multiple .CSV or .JDX files split from a map. For instructions, choose OMNIC Help Topics from the Help menu, find "CSV file format" in the Index and go to the "Opening a CSV text file" topic. The provided instructions apply to both .CSV and .JDX files.

1. **Choose Split Map from the Atlμs menu.**

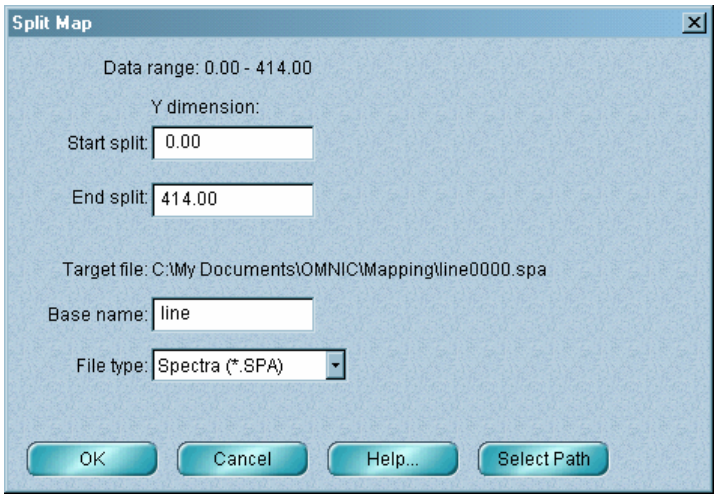
   The Split Map dialog box appears. If you are splitting an **area map**, it looks like this:



   The Data Range values indicate the ranges of the X and Y dimensions of the data in the map, respectively, in micrometers.

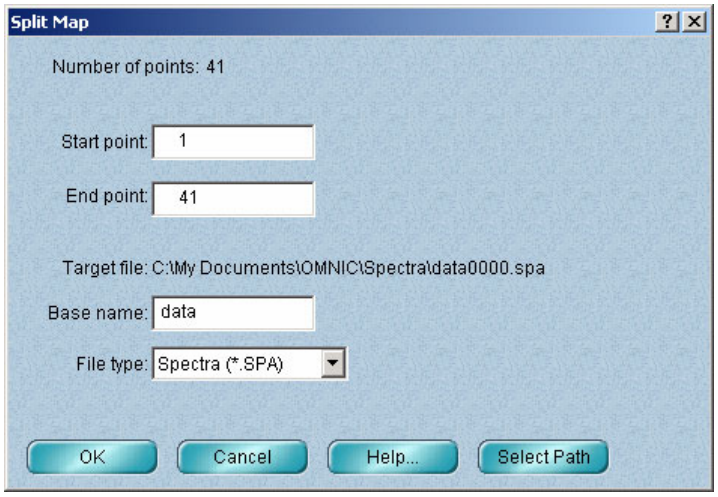
If you are splitting a *line map*, *line depth profile* or *area depth profile*, the dialog box looks like this:

For a depth profile the Z dimension is used instead of the Y dimension. It represents depth. A lower value indicates a shallower depth.



The Data Range values indicate the range of the distance dimension of the data in micrometers.

If you are splitting a *discrete point map*, the dialog box looks like this:



2. **Specify the starting and ending values of the portion of the map you want to split.**

   For an area map, type the starting and ending values for both the X and Y dimensions in the Start Split and End Split text boxes.

For a line map or depth profile, type the starting and ending values in the Start Split and End Split text boxes.

For a discrete point map, type the starting and ending values in the Start Point and End Point text boxes.

3. **Type a base name for saving the spectral data files in the Base Name text box.**

   The Target File readout shows the pathname that will be used for saving the files. The file name at the end consists of the specified base name, a four-digit number that will increase by one for each successive file saved, and an extension. Enter a unique, descriptive base name of up to four characters that will help you identify the files later.

4. **Specify the file type to use for the files by setting File Type.**

5. **Specify the directory that contains the map.**

   To do this, choose Select Path. The Select Path dialog box appears. Locate and select the directory; it should appear in the Look In box when you are finished. Then click the Select button.

6. **Choose OK.**

   The map is split into separate files, which are stored in the specified directory. This may take several minutes. After the map is split, a dialog box appears showing where the last file (and the preceding files) has been saved.

7. **Choose OK.**

   After you finish this procedure, you can start working with the new files using the features of OMNIC. For example, to open one of the new files, use Open in the File menu.

Quantifying a map

Use Quant Setup and Quantify in the Analyze menu to perform a quantitative analysis on a line map, area map or depth profile. The next sections explain how to specify a quant method using Quant Setup and quantify the map using Quantify.

Specifying a quant method

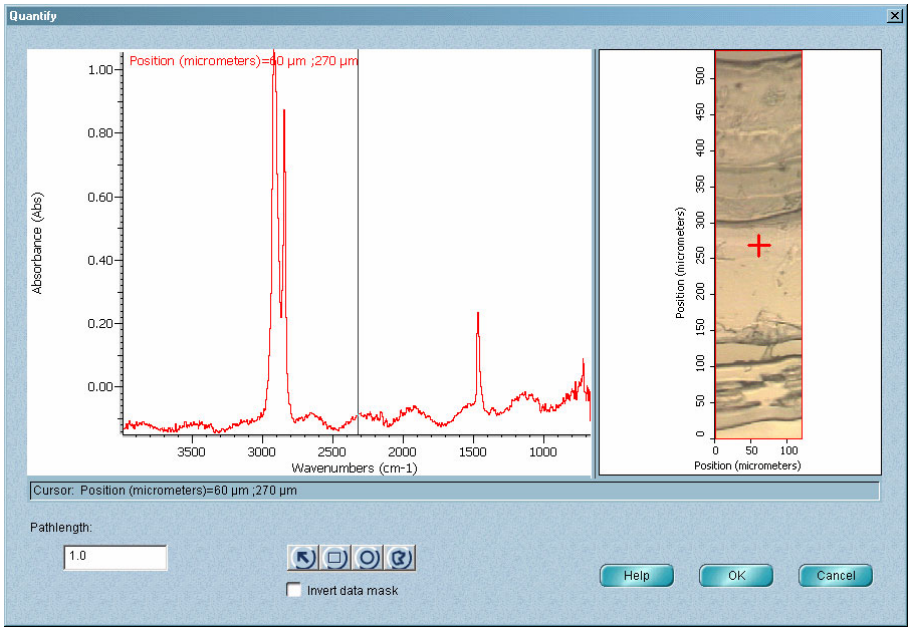
Use Quant Setup in the Analyze menu to specify a quant method for quantifying a line map or area map. In OMNIC Help Topics find "quant method" in the Index and go to "Selecting a quant method" for more information and instructions.

Quantifying the map

After you have specified a quant method with Quant Setup in the Analyze menu (see the preceding section), use Quantify in that menu to quantify the active line map, area map or depth profile. Follow these steps:

1. **Choose Quantify from the Analyze menu.**

   The Quantify window appears:



   The spectral display pane contains the spectrum collected at the point indicated by the cross hairs in the video image. You can display a different spectrum by using the arrow tool to click another point in the video image or drag the cross hairs. The location of the point appears below the spectral display pane.

You can zoom in on an area in the video image by drawing a box around the area in the video image and clicking inside the box. If desired, drag the handles on the sides or corners of the box to adjust its size and shape before clicking inside it.

You can zoom in on an area of the displayed spectrum by drawing a box around the area and clicking inside the box.

2. Type the pathlength in the Pathlength text box.

3. If you want to quantify only a portion of the spatial area of the map, specify the portion by using a mask.

You can select the rectangle mask tool by clicking it, or by *right-clicking* the video image and choosing Rectangle Mask Tool from the pop-up menu.

Several masks are available: To use a rectangular mask, select the rectangle mask tool and click the video image. A box appears:

Adjust the location, size and orientation of the box so that it surrounds the desired area. To move the box, point to its center and then drag the box. To resize the box, drag any side. To rotate the box, drag any corner.

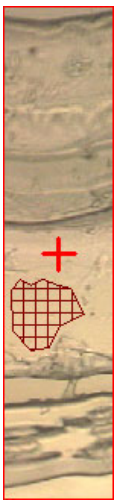
You can select the circle mask tool by clicking it, or by *right-clicking* the video image and choosing Circle Mask Tool from the pop-up menu.

To use a circular mask, select the circle mask tool and click the video image. A circle appears:

Adjust the location and size of the circle so that it surrounds the desired area. To move the circle, point to its center and then drag the circle. To resize the circle, drag its top or bottom or left or right side.

You can select the polygon mask tool by clicking it, or by *right-clicking* the video image and choosing Polygon Mask Tool from the pop-up menu.

To use a polygonal mask, select the polygon mask tool and click the location on video image where you want the polygon perimeter to start. Then click additional perimeter points to form the desired shape. Grid lines appear inside the polygon as you create it. To complete the polygon, either double-click the last perimeter point or click close to the starting point. Here is an example showing a completed polygon mask:



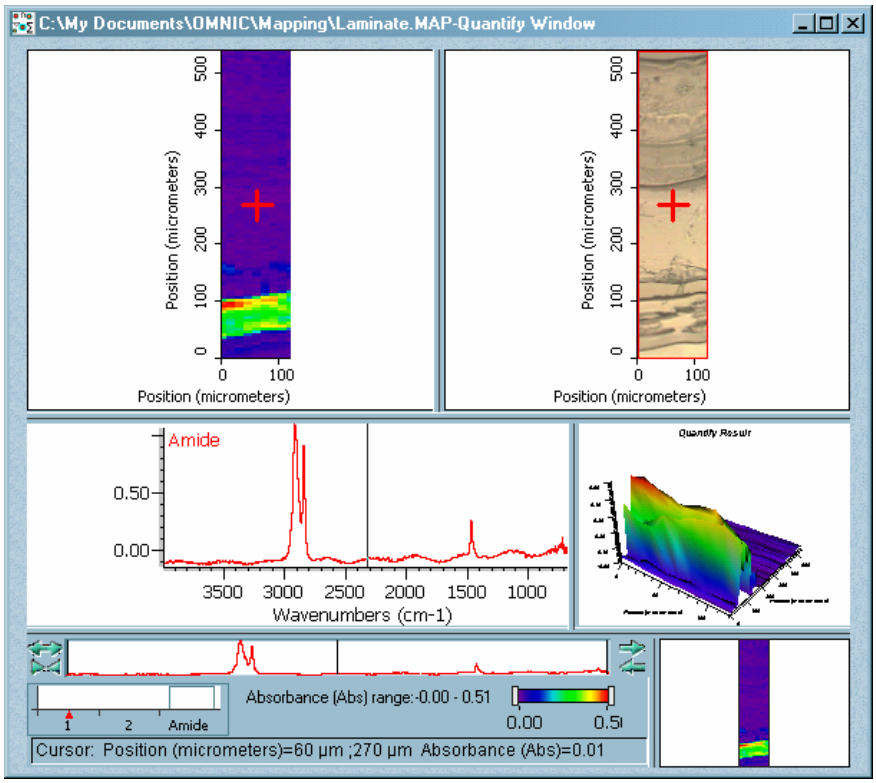
You can adjust the shape of the polygon by dragging a corner point or side of the polygon. To start over, draw a new polygon as explained above. The old polygon will be displayed in reverse video and then disappear.

You can use the area outside any mask shape for the analysis instead of the area inside the mask by selecting Invert Data Mask.

4. **Choose OK.**

The results appear in a new window:

You can change the size of the panes by dragging their borders.



You can use Display Setup to change how data is displayed in this window. See “Setting the display parameters” in the “Displaying Map Data” chapter for details.

The spectral display pane displays the spectrum collected at the point indicated by the cross hairs in the contour map (described below). You can display a different spectrum by clicking another point in the contour map or by dragging the cross hairs. You can display a different spectral region in this pane by using the view finder. For more information choose OMNIC Help Topics from the Help menu, find "view finder" in the Index and go to the "View finder" topic.

To display the results for a component measured by the quant method, click the desired component number near the lower-left corner of the window. The height of the box above each number indicates the concentration or other measured value of that component. When you point to a box, the value of that component appears.

Note The quant method determines which values are measured. The name of the quantitative analysis software used to develop the method was shown in the Origin box when you selected a method using Quant Setup. See the documentation that came with your quantitative analysis software for complete information on interpreting the analysis results. ▲

The results for the clicked component appear in the 3-D image and contour map, which show the relative distribution of the component across the sample surface. The vertical axis of the 3-D image indicates the concentration or other measured value of the component, as do the colors used in the 3-D image and contour map. You can adjust the distribution of the colors by adjusting the color bar just as you would in a map window. See "Using map windows" in the "Displaying Map Data" chapter for more information.

You can adjust the display of the 3-D image and contour map by using the sky view control just as you would in a map window. See "Using map windows" in the "Displaying Map Data" chapter if you need help.

You can print the entire window by using Print in the File menu. You can print individual panes by *right-clicking* the pane and choosing Print from the pop-up menu.

5. **To save the results in a map file that you can open later, choose Save Map As from the File menu.**

   See "Saving a map with a new file name or in a different location" in the "Saving and Exporting Map Data" chapter for instructions.

6. **To close the window, click the Close button (labeled "X") in the upper-right corner.**

   Depending on the quantitative analysis method you are using, you may be prompted to enter needed information. Follow the instructions that appear on the screen.

   If you want to find the locations of components in the sample, leave the window open and use RGB Display in the Atlμs menu. See "Finding components locations" for details.

Principal component analysis (PCA)

The next sections explain how to perform a principal component analysis and recalculate the results to reduce noise.

Performing a principal component analysis

Use Principal Component Analysis in the Atlμs menu to find the variance in an area map or area depth profile in terms of its principal components. The command reduces the dimensionality of the data set; that is, rather than looking at all of the spectral frequencies, you combine the information into a few values that describe the variation in the data.

The first principal component found describes the combination of spectral locations with the largest spectral variance in the map. The second principal component describes the second largest source of variance, and so on.

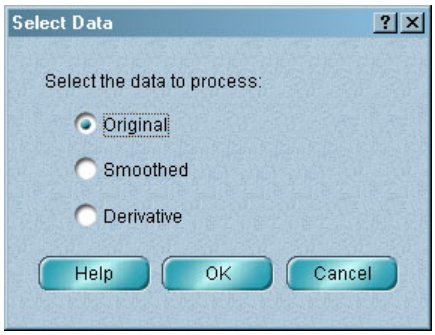
After you perform an analysis, you can use RGB Display in the Atlμs menu to blend specific results to find the locations of components in the sample. See "Finding component locations" for details.

You can reduce the noise in your PCA results by using PCA Recalculation in the Atlμs menu. See "Recalculating principal component analysis results" for details.

Follow these steps to perform a principal component analysis of the map in the active map window:

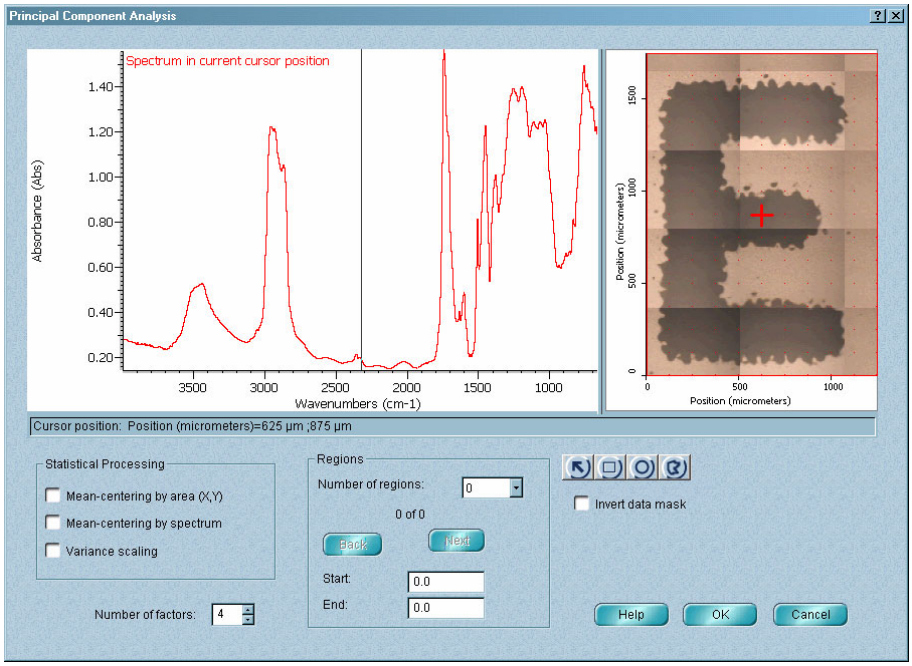
1. **Choose Principal Component Analysis from the Atlμs menu.**

   If you have processed the map using Smooth or Derivative in the Process menu and did not replace the original data with the processed data, a prompt appears. Here is an example:



Select the form of the data to use for the analysis and then choose OK. See “Smoothing map spectra by specifying the number of smoothing points” and “Converting map spectra to their first and second derivatives” for more information.

The Principal Component Analysis window appears:



The spectral display pane contains the spectrum collected at the point indicated by the cross hairs in the video image. You can display a different spectrum by using the arrow tool to click another point in the video image or drag the cross hairs. The location of the point appears below the spectral display pane.

You can zoom in on an area in the video image by drawing a box around the area in the video image and clicking inside the box. If desired, drag the handles on the sides or corners of the box to adjust its size and shape before clicking inside it. To redisplay the entire video image, *right-click* the image and then choose Full Range from the pop-up menu.

You can zoom in on an area of the displayed spectrum by drawing a box around the area and clicking inside the box. To redisplay the entire spectrum, *right-click* the spectrum and then choose Full Range from the pop-up menu.

2. **Select the desired options in the Statistical Processing box.**

   Mean-Centering By Area (X,Y) and Variance Scaling help remove effects that are unrelated to variation in chemical composition; for example, effects caused by variation in sample thickness or scattering.

   Mean-Centering By Spectrum helps remove effects caused by baseline variation.

3. **Set Number Of Factors to the desired number of principal components.**

   To change the setting, click the up or down arrow button.

4. **Use the features in the Regions box to specify the spectral regions for the analysis.**

   First specify the number of regions by setting Number Of Regions. If you select 0, the entire spectral range of the map will be used.

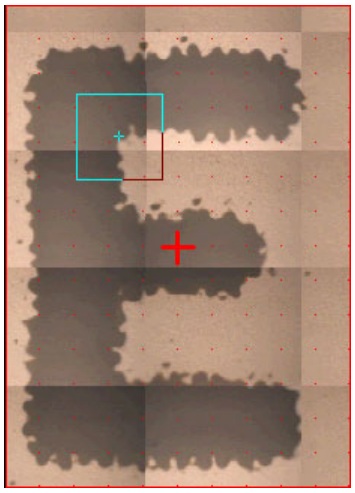
   Specify the limits of the first region by typing frequency values in the Start and End text boxes or by dragging the triangular region marker handles in the spectral display pane. The specified region is shaded.

   To specify the next region, click the Next button and then use the techniques described above. You can click the Back button to return to the settings for the previous region.

5. If you want to use only a portion of the spatial area of the map, specify the portion by using a mask.

You can select the rectangle mask tool by clicking it, or by *right-clicking* the video image and choosing Rectangle Mask Tool from the pop-up menu.

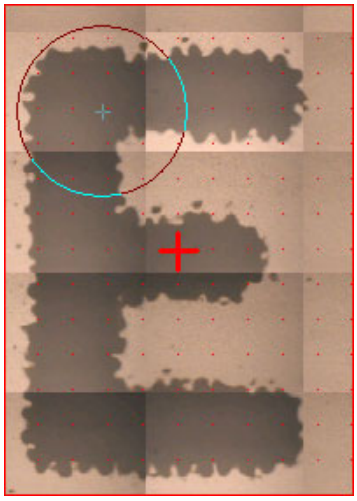
Several masks are available: To use a rectangular mask, select the rectangle mask tool and click the video image. A box appears:



Adjust the location, size and orientation of the box so that it surrounds the desired area. To move the box, point to its center and then drag the box. To resize the box, drag any side. To rotate the box, drag any corner.

You can select the circle mask tool by clicking it, or by *right-clicking* the video image and choosing Circle Mask Tool from the pop-up menu.

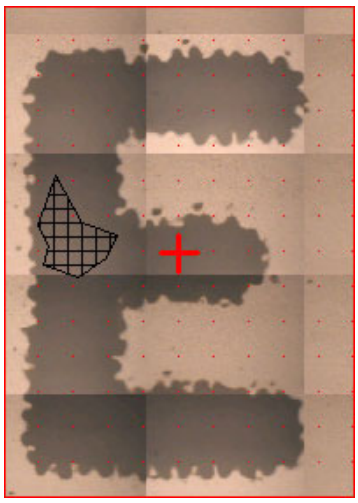
To use a circular mask, select the circle mask tool and click the video image. A circle appears:



Adjust the location and size of the circle so that it surrounds the desired area. To move the circle, point to its center and then drag the circle. To resize the circle, drag its top or bottom or left or right side.

You can select the polygon mask tool by clicking it, or by *right-clicking* the video image and choosing Polygon Mask Tool from the pop-up menu.

To use a polygonal mask, select the polygon mask tool and click the location on video image where you want the polygon perimeter to start. Then click additional perimeter points to form the desired shape. Grid lines appear inside the polygon as you create it. To complete the polygon, either double-click the last perimeter point or click close to the starting point. Here is an example showing a completed polygon mask:



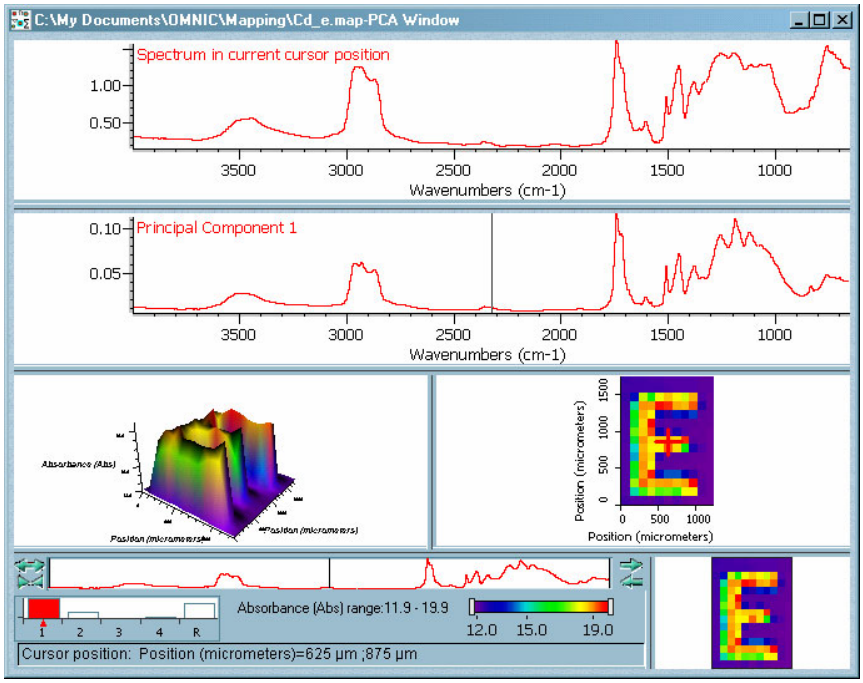
You can adjust the shape of the polygon by dragging a corner point or side of the polygon. To start over, draw a new polygon as explained above. The old polygon will be displayed in reverse video and then disappear.

If you saved a binary image as a mask during an image analysis and have not exited the software (the saved mask is still in memory), the Use Image Mask check box is available. If you select it, the portion of the map that corresponds to the black area of the saved mask will be used for the analysis. See “Performing an image analysis” in the “Analyzing Images” chapter for information about saving a binary image as a mask.

You can use the area outside any mask shape for the analysis instead of the area inside the mask by selecting Invert Data Mask.

6. Choose OK.

The analysis results appear in a new window:



You can change the size of the panes by dragging their borders.

You can use Display Setup to change how data is displayed in this window. See “Setting the display parameters” in the “Displaying Map Data” chapter for details.

The spectral display pane at the top of the window contains the spectrum collected at the point indicated by the cross hairs in the contour map (described below). You can display a different spectrum by clicking another point in the contour map or by dragging the cross hairs. You can display a different spectral region in this pane and in the principal component pane below it by using the view finder. For more information choose OMNIC Help Topics from the Help menu, find “view finder” in the Index and go to the “View finder” topic.

The principal component pane displays the principal components one at a time. Its vertical axis is used for the coefficient value, an indicator of relative contribution to spectral variance.

To display a component, click the desired component number near the lower-left corner of the window. The height of the box above each number indicates the overall relative strength of that component as a source of spectral variance. The first component is normally the strongest source. "R" represents the residual. If the box for the residual is large, it may indicate that additional components should be used in a new analysis.

The 3-D image shows the strength (measured along the vertical axis) of the current component over the mapped area of the sample.

The contour map is a two-dimensional representation of the strength of the current component over the mapped area. It shows which of the individual map spectra contribute the most to each of the sources of variance. Colors are used to indicate strength. You can adjust the distribution of the colors by adjusting the color bar just as you would in a map window. See "Using map windows" in the "Displaying Map Data" chapter for more information.

You can adjust the display of the 3-D image and contour map by using the sky view control just as you would in a map window. See "Using map windows" in the "Displaying Map Data" chapter if you need help.

7. **To save the analysis results in a map file that you can open later, choose Save Map As from the File menu.**

   See "Saving a map with a new file name or in a different location" in the "Saving and Exporting Map Data" chapter for instructions.

8. **To close the window, click the Close button (labeled "X") in the upper-right corner.**

   If you want to find the locations of components in the sample, leave the window open and use RGB Display in the Atlμs menu. See "Finding components locations" for details.

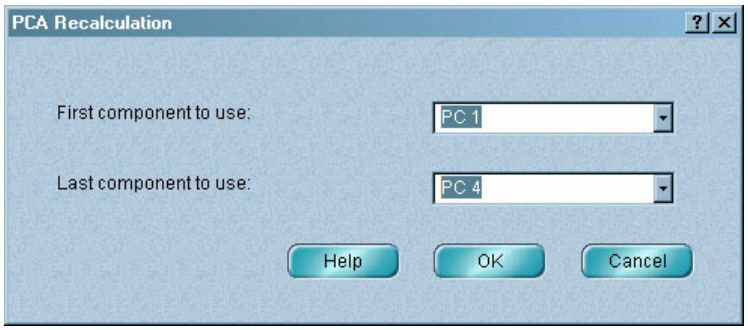
Recalculating principal component analysis results

Use PCA Recalculation in the Atlμs menu to improve the results of a principal component analysis by reducing noise contributed by particular components. See "Performing a principal component analysis" for information about using the Principal Component Analysis command.

Follow the steps below to use PCA Recalculation. The principal component analysis results must be displayed in the active window when you choose the command.

1. **Choose PCA Recalculation from the Atlμs menu.**

   The PCA Recalculation dialog box appears:



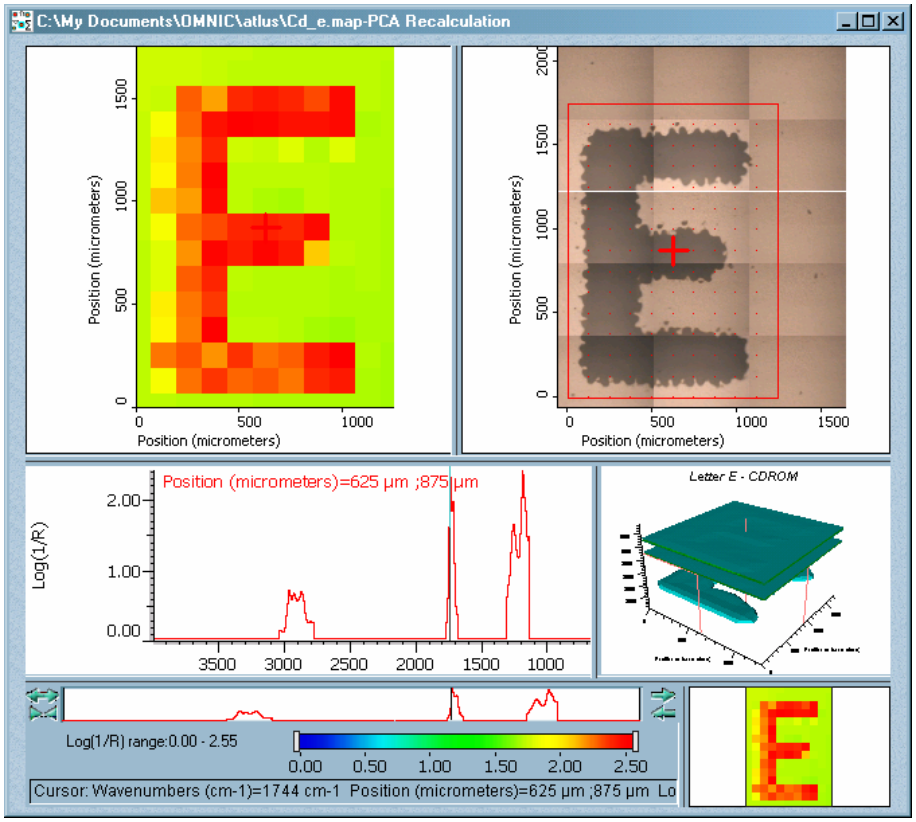
   This dialog box lets you specify the contiguous components to retain when the analysis is recalculated. By omitting one or more noisy components (or the residual) at the beginning and end of the sequence, you can produce a result with less noise.

2. **Specify the first component to retain by setting First Component To Use.**

3. **Specify the last component to retain by setting Last Component To Use.**

4. **Choose OK.**

   The analysis results appear in a new window:



   This window is very similar to a map window. See "Using map windows" for information about manipulating the parts of the window.

   You can change the size of the panes by dragging their borders.

5. **To save the results in a map file that you can open later, choose Save Map As from the File menu.**

   See "Saving a map with a new file name or in a different location" in the "Saving and Exporting Map Data" chapter for instructions.

6. **To close the window, click the Close button (labeled "X") in the upper-right corner.**

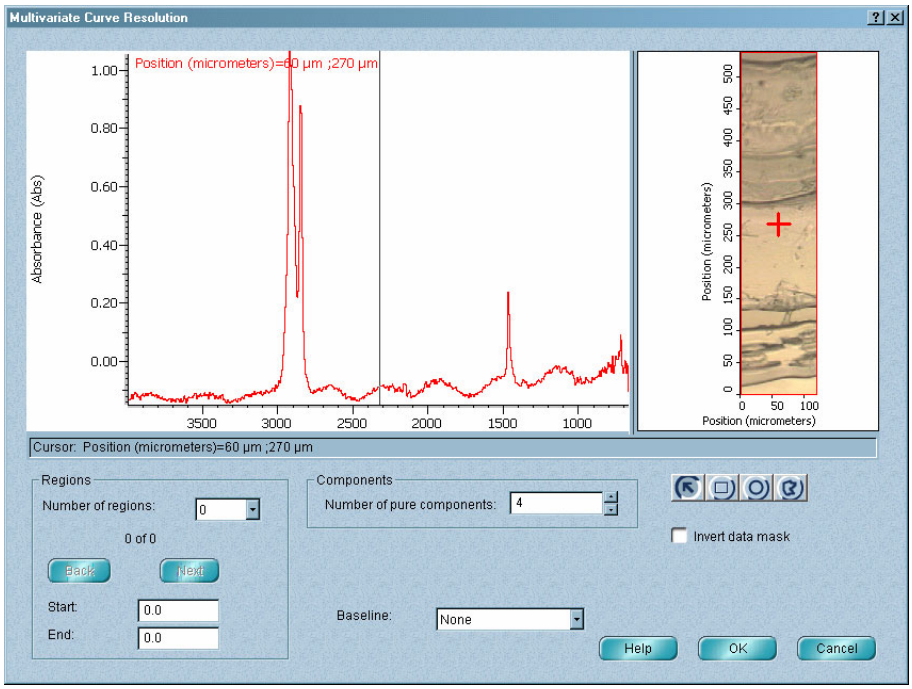
Using Multivariate Curve Resolution

Multivariate Curve Resolution (MCR) lets you estimate which pure components are present in the active area map or area depth profile, as well as the locations and concentrations of those components. This is an enhancement over normal map analysis, since the estimates of the pure components and the concentrations are computed at the same time. Also, unlike the principal components that result from principal component analysis (PCA), the pure component spectra that result from MCR can be searched against spectral databases.

Follow these steps to use MCR:

1. **Choose Multivariate Curve Resolution from the Atlμs menu.**

   The Multivariate Curve Resolution window appears:



   The spectral display pane contains the spectrum collected at the point indicated by the cross hairs in the video image. You can display a different spectrum by using the arrow tool to click another point in the video image or drag the cross hairs. The location of the point appears below the spectral display pane.

Note The displayed spectrum does not affect the MCR calculation. It only helps you define the spectral regions to use for the calculation. ▲

You can zoom in on an area in the video image by drawing a box around the area in the video image and clicking inside the box. If desired, drag the handles on the sides or corners of the box to adjust its size and shape before clicking inside it. To redisplay the entire video image, *right-click* the image and then choose Full Range from the pop-up menu.

You can zoom in on an area of the displayed spectrum by drawing a box around the area and clicking inside the box. To redisplay the entire spectrum, *right-click* the spectrum and then choose Full Range from the pop-up menu.

2. **Use the features in the Regions box to specify the spectral regions for the analysis.**

   First specify the number of regions by setting Number Of Regions. If you select 0, the entire spectral range of the map will be used.

   Specify the limits of the first region by typing frequency values in the Start and End text boxes or by dragging the triangular region marker handles in the spectral display pane. The specified region is shaded.

   To specify the next region, click the Next button and then use the techniques described above. You can click the Back button to return to the settings for the previous region.

3. **Specify the number of components to quantify.**

   You can type a number from 1 to 10 in the Number Of Pure Components text box or click the up and down arrow buttons to the right.

Note MCR requires a large amount of computer processing power and speed. Depending on its capability, your computer may not be able to calculate more than four or five components. We recommend starting with a small number of components and increasing the number in increments of one. ▲

4. **Specify an algorithm by setting Baseline.**

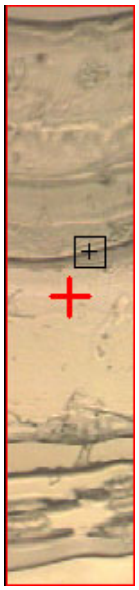
   The available algorithms, described in the table below, prevent the data from dropping below a zero baseline (Y values are always positive). Select None if you don't want to ensure positive Y values.

Setting	Description
None	The baseline is allowed to drop below zero.
Constant	A constant baseline is added as a "component" for each spectrum. This baseline value is determined along with the amount of each component.
Linear	Two "components" are added for each spectrum. One is the constant part of the linear baseline, and the other is the sloping part of the linear baseline.
Quadratic	Three "components" are added for each spectrum. One is the constant part of the quadratic baseline, the second is the sloping part of the quadratic baseline, and the third is the curved part of the quadratic baseline.

5. If you want to use only a portion of the spatial area of the map, specify the portion by using a mask.

You can select the rectangle mask tool by clicking it, or by *right-clicking* the video image and choosing Rectangle Mask Tool from the pop-up menu.

Several masks are available: To use a rectangular mask, select the rectangle mask tool and click the video image. A box appears:



Adjust the location, size and orientation of the box so that it surrounds the desired area. To move the box, point to its center and then drag the box. To resize the box, drag any side. To rotate the box, drag any corner.

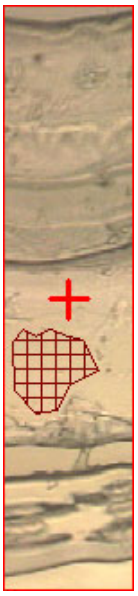
You can select the circle mask tool by clicking it, or by *right-clicking* the video image and choosing Circle Mask Tool from the pop-up menu.

To use a circular mask, select the circle mask tool and click the video image. A circle appears:

Adjust the location and size of the circle so that it surrounds the desired area. To move the circle, point to its center and then drag the circle. To resize the circle, drag its top or bottom or left or right side.

You can select the polygon mask tool by clicking it, or by *right-clicking* the video image and choosing Polygon Mask Tool from the pop-up menu.

To use a polygonal mask, select the polygon mask tool and click the location on video image where you want the polygon perimeter to start. Then click additional perimeter points to form the desired shape. Grid lines appear inside the polygon as you create it. To complete the polygon, either double-click the last perimeter point or click close to the starting point. Here is an example showing a completed polygon mask:



You can adjust the shape of the polygon by dragging a corner point or side of the polygon. To start over, draw a new polygon as explained above. The old polygon will be displayed in reverse video and then disappear.

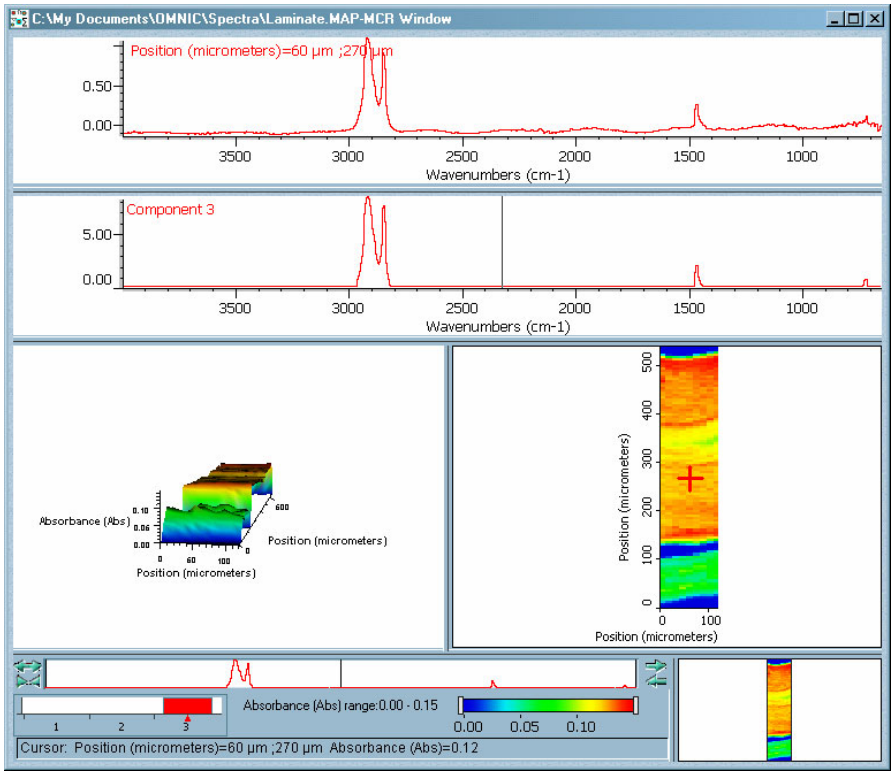
If you saved a binary image as a mask during an image analysis and have not exited the software (the saved mask is still in memory), the Use Image Mask check box is available. If you select it, the portion of the map that corresponds to the black area of the saved mask will be used for the analysis. See “Performing an image analysis” in the “Analyzing Images” chapter for information about saving a binary image as a mask.

You can use the area outside any mask shape for the analysis instead of the area inside the mask by selecting Invert Data Mask.

6. Choose OK.

The analysis results appear in a new window. Here is an example:

You can change the size of the panes by dragging their borders.



You can use Display Setup to change how data is displayed in this window. See “Setting the display parameters” in the “Displaying Map Data” chapter for details.

The spectral display pane at the top of the window contains the spectrum collected at the point indicated by the cross hairs in the contour map (described below). You can display a different spectrum by clicking another point in the contour map or by dragging the cross hairs. You can display a different spectral region in this pane and in the principal component pane below it by using the view finder. For more information choose OMNIC Help Topics from the Help menu, find “view finder” in the Index and go to the “View finder” topic.

The component pane displays the components one at a time. Its vertical axis is used for the coefficient value, which is proportional to the concentration.

To display a component, click the box above the desired component number near the lower-left corner of the window. The height of the box indicates the relative portion of the total composition attributed to that component. When you point to a box, the portion is shown as a numerical value.

The 3-D image shows the relative concentration (measured along the vertical axis) of the current component over the mapped area of the sample.

The contour map is a two-dimensional representation of the relative concentration of the current component over the mapped area. Colors are used to indicate concentration. You can adjust the distribution of the colors by adjusting the color bar just as you would in a map window. See "Using map windows" in the "Displaying Map Data" chapter for more information.

You can adjust the display of the 3-D image and contour map by using the sky view control just as you would in a map window. See "Using map windows" in the "Displaying Map Data" chapter if you need help.

7. **To save the analysis results in a map file that you can open later, choose Save Map As from the File menu.**

   See "Saving a map with a new file name or in a different location" in the "Saving and Exporting Map Data" chapter for instructions.

8. **To close the window, click the Close button (labeled "X") in the upper-right corner.**

   If you want to find the locations of components in the sample, leave the window open and use RGB Display in the Atlμs menu. See "Finding components locations" for details.

Finding component locations

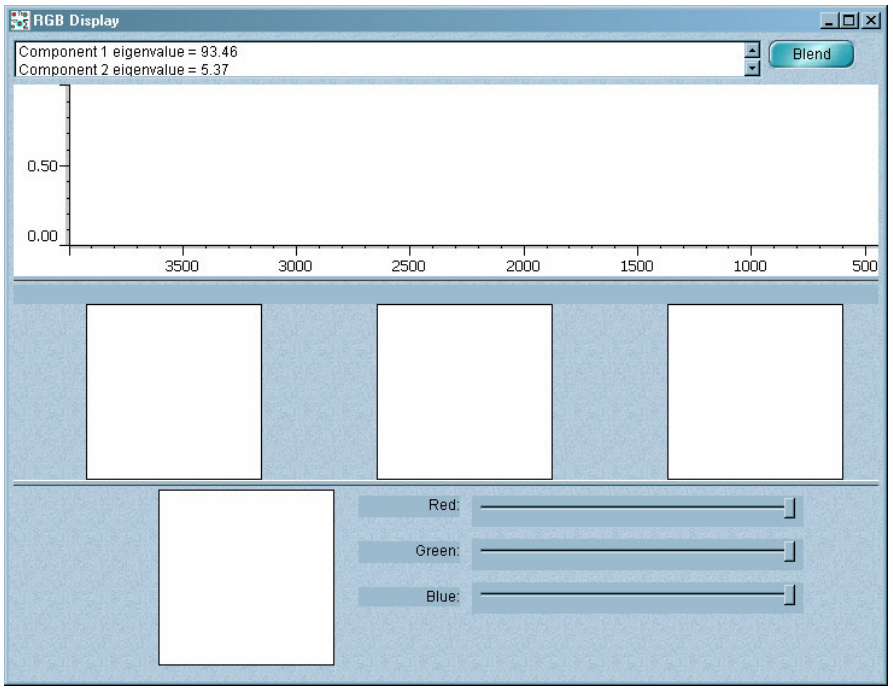
Use RGB Display in the Atlμs menu to blend specific analysis results to find the physical locations of components in the sample. You can this command after you perform a principal component analysis (or open saved results), use Multivariate Curve Resolution (or open saved results), or quantify a map. See “Performing a principal component analysis,” “Using Multivariate Curve Resolution” or “Quantifying the map” for information about performing the mentioned operations.

Follow the steps below to use RGB Display. The results of using Principal Component Analysis, Multivariate Curve Resolution or Quantify must be displayed in the active window when you choose the command.

1. **Choose RGB Display from the Atlμs menu.**

   The RGB Display window appears:

The spectral display pane does not appear for quantitative analysis results.



2. **Select up to three items to blend from the list of items near the top of the window.**

   The list includes the principal components and the residual. To select an item, click it. If you change your mind, click the item again.

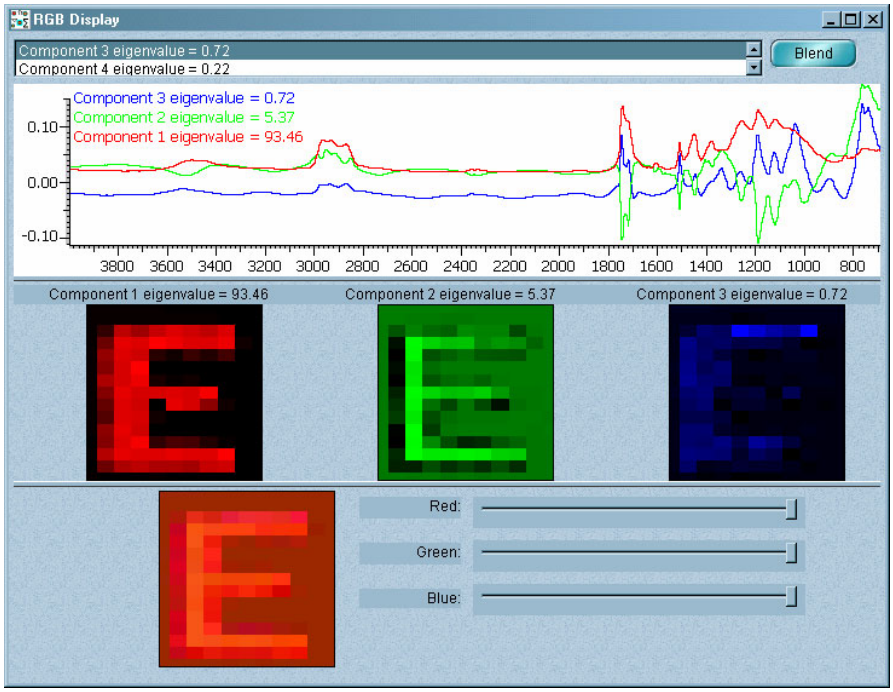
Click the up and down arrow buttons as needed to bring items into view in the box.

The selected items are overlaid in the top pane (see the illustration in the next step). The vertical axis of the pane indicates the relative contribution of the component to the spectral variance.

You can change the height of the top pane and the others by dragging their borders up or down as desired.

3. Click the Blend button.

A contour map of each selected item appears in the center pane of the window, with red, green and blue used to display the first, second and third maps, respectively. The name of the component or residual appears above each map. The pattern of color in a map indicates how the strength of the component is distributed across the area of the map. Here is an example:



A blended image of the selected items appears in the bottom pane. The colors in the blended image result from adding together the colors of the selected images.

The Red, Green and Blue controls to the right of the blended image let you adjust the intensity of the colors. Simply drag the small vertical bars to the left or right.

4. **To save the results in the same file that contains the principal component analysis results, choose Save Map As from the File menu.**

   See "Saving a map with a new file name or in a different location" in the "Saving and Exporting Map Data" chapter for instructions.

Note You can copy the contents of the bottom four panes by *right-clicking* the pane and choosing Copy from the pop-up menu. ▲

5. **To close the window, click the Close button (labeled "X") in the upper-right corner.**

Analyzing Images

The Image Analysis command in the Atlμs menu lets you set up and perform "feature sizing," a type of analysis in which you measure, count or identify features in a chemical image (two-dimensional contour map) or video image. You can use the analysis to determine…

- The distribution of chemical or visual features on or in a sample.
- The size of the features.
- The percentage of the mapped portion of the sample that the features occupy.

The next sections describe the filters you can use in an analysis and the morphology options you can select. Then "Performing an image analysis" provides a step-by-step image analysis procedure.

Using gray scale filters

When you choose Image Analysis from the Atlμs menu, the software converts the full-color chemical or video image into a gray scale image and displays it in the Image Analysis window. You can enhance this image by applying gray scale filters, available through the Filter Setup button on the Filters tab. The filters belong to classes whose names indicate their general purpose. The table below describes the available filters. Refer to this table when selecting filters during the procedure in "Performing an image analysis" later in this chapter.

Class	Filter	Description
Smoothing	Mean	Convolution filter that replaces every pixel with the average value of all the pixels within the convolution kernel. It also reduces the level of the salt-and-pepper (impulse) noise.
	Weighted Mean	Convolution filter with different coefficients in the convolution kernel that give more importance (weight) to central pixels within the convolution neighborhood. The result of this convolution is less blurred than that of the Mean filter. It also reduces the level of the salt-and-pepper (impulse) noise. Also known as Lowpass and Gaussian filters. When you select this filter, the Set button becomes available in the Advanced column in the Image Processing Setup dialog box. When you click the button, the Advanced Options For Weighted Mean Filter dialog box appears. Set the averaging coefficient and choose OK.
	Adaptive Mean	Convolution filter that is similar to the Mean filter, except that a pixel is used to compute the mean if, and only if, the difference between that pixel and the center pixel is less than or equal to the specified maximum difference. The result of this convolution is less blurred than that of the Mean filter. It also reduces the level of high-frequency (salt-and-pepper) noise. When you select this filter, the Set button becomes available in the Advanced column in the Image Processing Setup dialog box. When you click the button, the Advanced Filter Options dialog box appears. Set the maximum difference for the filter and choose OK.
	Open	Nonlinear filter that computes the morphological erosion followed by the dilation using a circular structuring element as the kernel. It removes small low-intensity (dark) features and smoothes the edges.

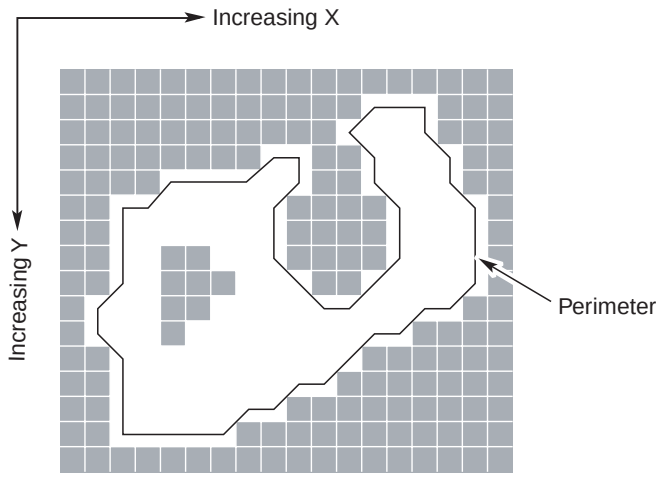
Class	Filter	Description
	Close	Nonlinear filter that computes the morphological dilation followed by the erosion using a circular structuring element as the kernel. It removes small high-intensity (bright) features and smoothes the edges.
Noise Removal	Rank	Nonlinear filter whose response is based on ordering (ranking) the pixels within the kernel and then replacing the central pixel with a value from the ranking. It effectively cancels evenly distributed salt-and-pepper (impulse) noise and reduces gray-level oscillations without blurring. However, it may shift the edges of the image. When you select this filter, the Set button becomes available in the Advanced column in the Image Processing Setup dialog box. When you click the button, the Advanced Filter Options dialog box appears. Set the rank difference percentage and choose OK.
	Median	Special case of the Rank filter (see the description above) that uses the median value for the pixel result.
	Open	See the description in the Smoothing class.
	Close	See the description in the Smoothing class.
Sharpening	High-boost	Convolution filter that enhances differences in gray levels. It acts like a Laplace edge enhancement added back to the original image. When you select this filter, the Set button becomes available in the Advanced column in the Image Processing Setup dialog box. When you click the button, the Advanced Options For High-boost Filter dialog box appears. Set the filter coefficients and choose OK.
	Gated Rank	Similar to the Rank filter but uses two percentile values: low and high gate values. The result central pixel in the kernel neighborhood will be either the low or high gate value, whichever is closer to the value of the central pixel. Tends to make spatial areas more evenly distributed, also canceling some noise. When you select this filter, the Set button becomes available in the Advanced column in the Image Processing Setup dialog box. When you click the button, the Advanced Filter Options dialog box appears. Set the low rank and high rank percentages and choose OK.

Class	Filter	Description
	MinMax	Special case of the Gated Rank filter that replaces the central pixel with either the minimum or maximum value from the kernel neighborhood, whichever is closer to the intensity of the center. Tends to enlarge and smooth the brightest and darkest areas in an image without changing intermediate areas. Also cancels some impulse noise. When you select this filter, the Set button becomes available in the Advanced column in the Image Processing Setup dialog box. When you click the button, the Advanced Filter Options dialog box appears. Set the rank difference percentage and choose OK.
Edge Detection	Sobel	Two-pass convolution filter that enhances edges and small areas where intensity changes. Also blanks large areas with constant intensity. Useful for defect inspection.
	Morph Gradient	Computed as the difference between the morphological dilation and erosion with a circular structuring element. Highlights sharp gray-level transitions in the input image.
	Laplace	Convolution filter that enhances image edges and small areas where intensity changes. Also blanks large areas with constant intensity. Useful for defect inspection. When you select this filter, the Set button becomes available in the Advanced column in the Image Processing Setup dialog box. When you click the button, the Advanced Options For Laplace Filter dialog box appears. Select the desired coefficients and choose OK.
Contrast Adjustment	Histogram Stretch	Enhances the contrast in the significant portion of the image; that is, where the histogram peak intensities exceed a specified threshold. This filter is useful when a sharpening filter has produced an image whose important areas have low contrast. When you select this filter, the Histogram Stretching dialog box appears. Specify a clip threshold by typing a percentage value from 0.1 to 10 in the text box or by using the slider. Peaks that are less than the specified percentage of the maximum peak value are reduced to zero. Peaks that are within the specified percentage of the maximum peak value are increased to the maximum value. The range of values of the remaining peaks is "stretched" to go from zero to the maximum value. Choose OK to apply the filter.

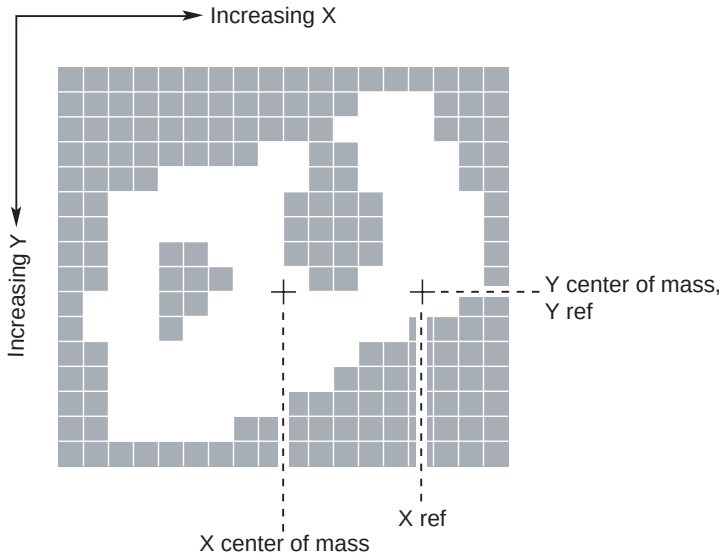
Note If you set Filter Class to All Filters, all of the filters listed above become available. ▲

Morphology options

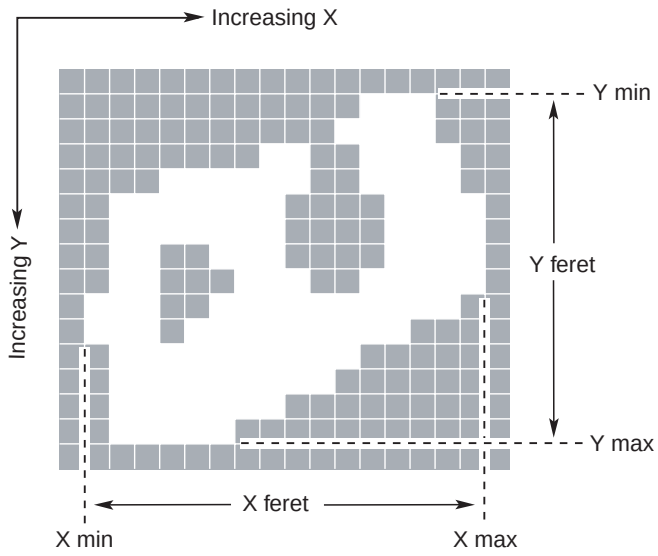
Morphology refers to the size, shape and measurements of the image features you want to size. The table below describes the histogram parameters that become available when you select feature parameters on the Morphology tab (available through the Setup button on the Feature Sizing tab). Where appropriate, illustrations convey the meaning of the histogram parameters using an example image. Refer to this table when setting morphology options during the procedure in "Performing an image analysis" later in this chapter.

Selected Feature Parameter	Available Histogram Parameters	Description
Area	Area	Feature area, as the number of pixels in the feature times pixel area, in current units squared. At the bottom of the results table, three additional values appear: Total Image Area is the area of the entire image. Total Feature Area is the sum of the areas of the measured features. Feature Area Percentage is the percentage of the total image area that is within the measured features.
Dimensional	Perimeter	Sum of the distances between centers of adjacent pixels on the feature perimeter, times pixel width, in current units. 
	Circularity	Perimeter squared divided by (4 pi times pixel area).

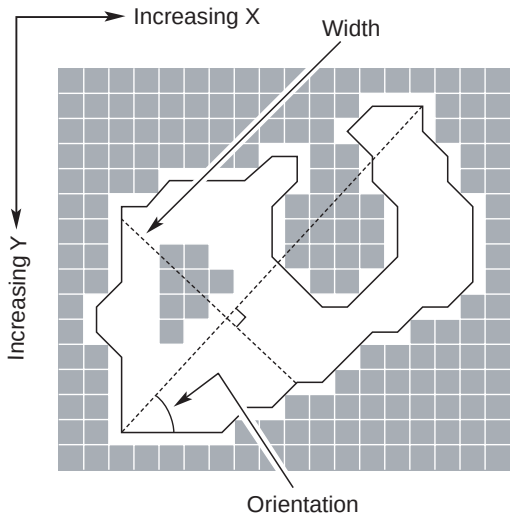
Selected Feature Parameter	Available Histogram Parameters	Description
Location	X Center Of Mass	X center of mass, as the average value of feature pixel X coordinate.
	Y Center Of Mass	Y center of mass, as the average value of feature pixel Y coordinate. See the preceding illustration.
	X Ref	To define the X Ref value, the software searches all horizontal chords along the Y center of mass to find the center of the largest horizontal chord. See the preceding illustration.
	Y Ref	True center of mass. See the preceding illustration.

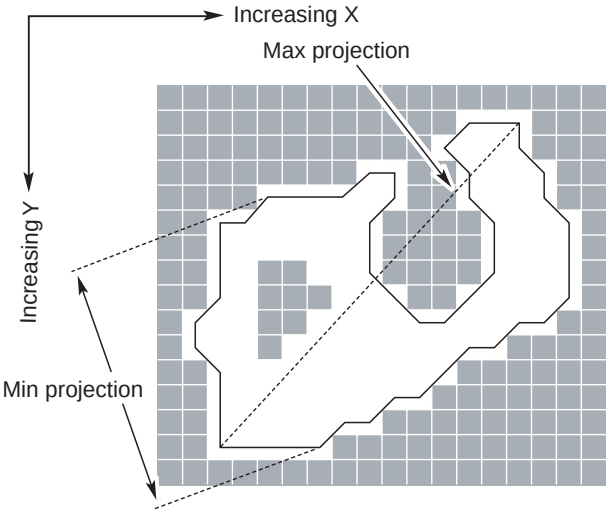


Selected Feature Parameter	Available Histogram Parameters	Description
Feret	X Feret	Projection of the feature on the X-axis.
	Y Feret	Projection of the feature on the Y-axis. See the preceding illustration.
	X Min	Minimum value of the feature pixel X coordinate. See the preceding illustration.
	X Max	Maximum value of the feature pixel X coordinate. See the preceding illustration.
	Y Min	Minimum value of feature pixel Y coordinate. See the preceding illustration.
	Y Max	Maximum value of the feature pixel Y coordinate. See the preceding illustration.
Fiber/Stringer	Length	Derived length of the feature or fiber, after it is straightened into a rectangle of equal area and perimeter, in current units.

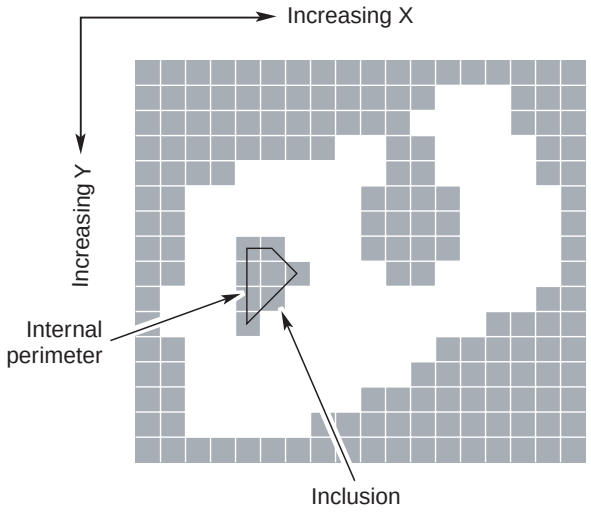


Selected Feature Parameter	Available Histogram Parameters	Description
	Width	Feature projection perpendicular to the maximum projection, in current units.
	Aspect Ratio	Maximum projection divided by pixel width. Unitless.
	Orientation	Angle between the positive X-axis and the maximum feature projection, in degrees. Clockwise rotation from the X-axis is a positive orientation angle. See the preceding illustration.
Projections	Max Projection	Maximum feature projection (maximum caliper dimension), as the largest separation between points on the feature convex perimeter, in current units.

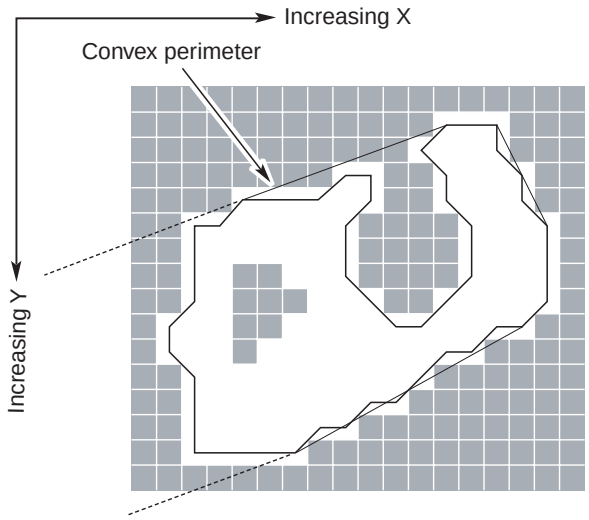




Selected Feature Parameter	Available Histogram Parameters	Description
	Min Projection	Minimum feature projection (minimum caliper dimension), as the smallest separation between points on the feature convex perimeter, in current units. See the preceding illustration.
	Mean Projection	Minimum feature projection (minimum caliper dimension), as the shortest altitude of all triangles drawn between pixels on the convex perimeter, in current units. Triangle bases are defined by adjacent pixels, and peaks by pixels on the opposite side of the feature.
	Standard Deviation	Standard deviation of the projection measurements.
Internal	Internal Perimeter	Internal perimeter, as the sum of distances between centers of adjacent pixels on the perimeters of feature inclusions, times pixel width, in current units.
	Internal Area	The number of non-feature pixels completely surrounded by feature pixels multiplied by pixel area, in current units squared.
	Internal Count	The number of discrete inclusions.
Convex	Convex Area	Convex area, as the number of pixels inside the feature convex perimeter, times pixel area, in current units.
	Convex Circularity	Convex circularity, as convex perimeter squared, divided by (4 pi times convex area). Unitless.



Selected Feature Parameter	Available Histogram Parameters	Description
	Convex Length	Convex length, derived as the length of a feature or fiber after it is straightened into a rectangle of equal area and perimeter, in current units.
	Convex Perimeter	Convex perimeter, as the sum of distances between centers of adjacent pixels on the feature convex perimeter, times pixel width, in current units.



Performing an image analysis

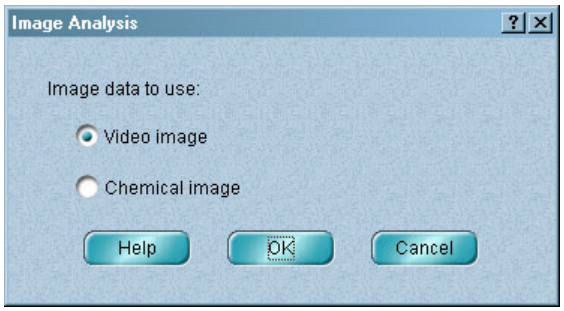
When you perform an image analysis, you first specify filters and intensity thresholds to designate the features of interest in the video image or chemical image (two-dimensional contour map). You then perform feature sizing to obtain information about the size and distribution of these features. You can perform an analysis on an image displayed in a map window, profile window, PCA results window or MCR results window. Follow these steps:

1. **Display the portion of the data that you want to analyze.**

   See "Zooming in and out on map data" or "Adjusting the display with the sky view control" in the "Displaying Map Data" chapter for information on displaying only a portion of the data.

2. **Choose Image Analysis from the Atlμs menu.**

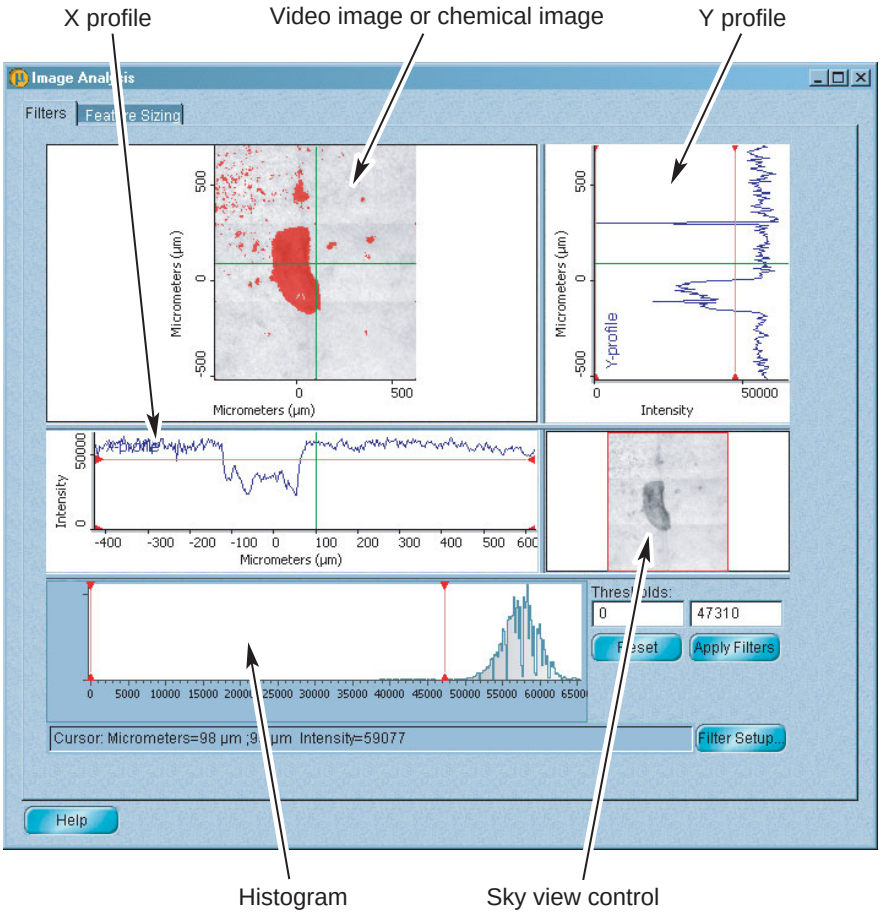
   The Image Analysis dialog box appears:



3. **Select the type of image you want to analyze and then choose OK.**

Note The Chemical Image option is not available for line maps or line depth profiles. ▲

The Image Analysis window appears, with the Filters tab in front:



You can change the sizes of the panes by dragging the borders that separate them.

The Filters tab lets you define and view profiles that show image intensity along the image cross hairs. For a video image, this is the gray level intensity; for a chemical image, this is the spectral intensity.

Each profile pane shows the image intensity along the corresponding cross hair in the image. You can move the cross hairs by dragging them or clicking a new location. The coordinate values of the current location appear below the histogram.

The image pixels whose intensity falls within the intensity thresholds appear in red. You can adjust the thresholds by dragging the red threshold lines in either profile pane or in the histogram. You can also set the thresholds numerically by typing values in the Thresholds text boxes.

To reset the thresholds to their original values (or to values determined by Auto-threshold in the Filter Setup dialog box, as explained in the next step), click the Reset button.

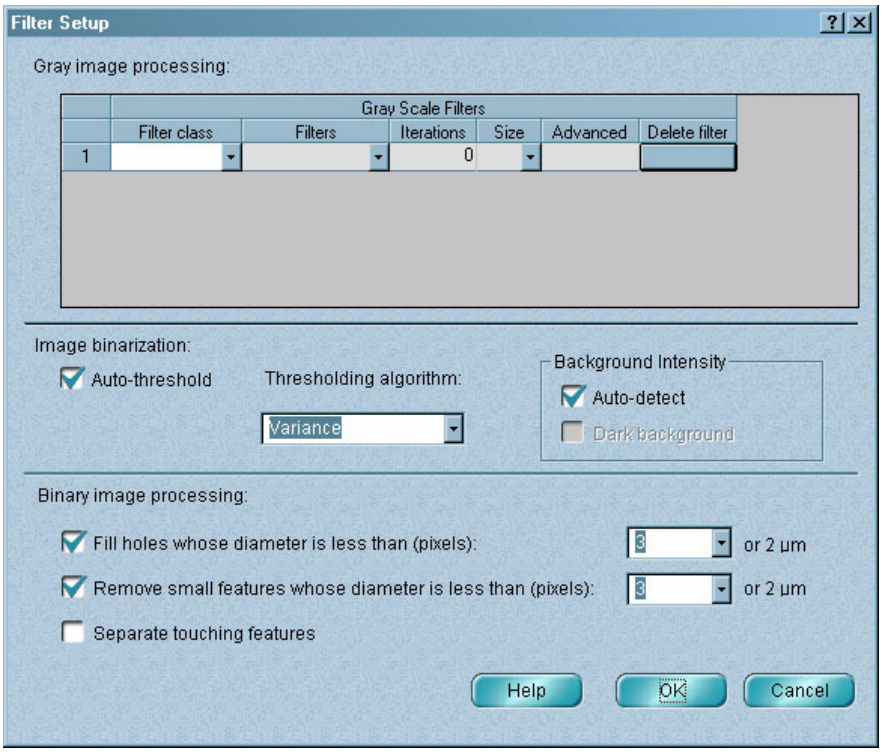
By adjusting the thresholds and using optional gray scale filters (explained in the next step), you designate the pixels that make up the features to be analyzed on the Feature Sizing tab. These pixels will appear in black in the binary image displayed on that tab.

The histogram shows the relative distribution of the intensity values of the image pixels. (The X-axis is in intensity units.) Darker shades of gray are used in the histogram to represent lower intensities, and lighter shades represent higher intensities. These shades correspond to the shades found in the image.

4. **If you want to specify filters that can enhance the image and let you locate features of interest, click the Filter Setup button.**

Note This step should be performed only if you need to enhance the image by smoothing it, sharpening it or removing noise. If you skip this step, continue with step 5. ▲

When you click the button, the Filter Setup dialog box appears:



At the top of the dialog box is a table that lets you specify gray scale filters to use for the analysis. The available filters are grouped into filter classes. See "Using gray scale filters" earlier in this chapter for descriptions of the filters in each class. Follow these steps to add or change the settings for a filter:

a. Select the desired class from the drop-down list box in the appropriate row in the Filter Class column. The filters in that class become available.

b. Select the desired filter from the drop-down list box in the Filters column.

c. Specify the number of times to apply the filter by typing a number in the Iterations column. Normally one iteration is enough.

d. Select the desired kernel size (3-by-3 or 5-by-5) from the drop-down list box in the Size column. The kernel is a matrix of pixels that will be passed over each pixel in the image. The intensity of the pixel under the kernel is replaced by the sum of each pixel intensity in the kernel times the coefficient value of the corresponding kernel pixel. Depending on the filters you have specified, the coefficient values can be positive or a mixture of positive and negative.

e. If the Set button is available in the Advanced column, click the button if you want to set advanced options for the filter. The Advanced Filter Options dialog box appears. Set the provided options and choose OK.

To delete a filter from the table, click the Delete button in the filter's row in the Delete Filter column.

Binarization classifies the gray-level image pixels as either foreground or background, based on a calculated threshold. If you want the software to automatically calculate the optimal threshold, select Auto-threshold. This is often gives a good starting point for binarization. (You can still adjust the thresholds more precisely on the Filters tab using the techniques explained in the preceding step.) Specify a thresholding algorithm by setting Thresholding Algorithm. The following table describes the optimization criteria of available algorithms:

Setting	Description
Variance	Minimizes the ratio of between-class variance to within-class variance for the bright and dark classes. This works best when the histogram has two or more peaks.
Entropy	Calculates the optimal threshold that maximizes the sum of the information (Shannon) entropies of the bright and dark classes. This works even if the histogram has only one pronounced peak (that is, a unimodal histogram).

Setting	Description
Moments	Calculates the threshold based on preserving the statistical moments in the histogram. This is the fastest algorithm, since it has a direct formula for the threshold position.

Features can appear as either dark areas on a light background, or light areas on a dark background. If you want the software to automatically determine whether the background is light or dark, select Auto-detect in the Background Intensity box. In this case the software assumes that most of the image area is background. If less than half of image area is background, do not use Auto-detect. Instead, examine the image to determine whether the background is light or dark. If it is dark, select Dark Background; if it is light, make sure Dark Background is not selected.

To fill "holes" in features so that the features appear solid, select Fill Holes Whose Diameter Is Less Than (Pixels) and select the desired hole size threshold, in pixels, from the drop-down list box to the right. The equivalent size in micrometers appears to the right. You can also type a value in the text box. The largest dimension of each hole will be used to determine whether the hole is filled. Select All if you want all holes, regardless of size, to be filled.

To delete small features, select Remove Small Features Whose Diameter Is Less Than (Pixels) and select the desired feature size threshold, in pixels, from the drop-down list box to the right. You can also type a value in the text box. The largest dimension of each feature will be used to determine whether the feature is deleted.

To create a small gap between features that are connected, select Separate Touching Features.

5. Choose OK to close the Filter Setup dialog box.

The effects of your settings appear on the Filters tab.

6. Work with the displayed data and image as desired.

If you change threshold values to improve the binarization and want to reapply the previously specified filters (see step 3), click the Apply Filters button.

You can measure items in the image: *Right-click* the image, point to Cursor Mode, choose Ruler from the pop-up menu, and then drag across the image to draw a ruler. The measured distance appears below the histogram. You can manipulate the ruler just as you would in the Atlμs window. See "Moving the ruler" and "Resizing the ruler" in the "Preparing for Data Collection" chapter if you need help. To remove the ruler, *right-click* the map, point to Cursor Mode and choose Select And Zoom from the pop-up menu.

When the ruler is not being used, you can zoom in on an area of interest by drawing a box on the image or in a profile pane and clicking inside the box, just as you would in a map window. See "Zooming in and out on map data" in the "Displaying Map Data" chapter for details.

You can use the sky view control to change the display of the image just as you would to adjust the display of data in a map window. For details see "Adjusting the display with the sky view control" in the "Displaying Map Data" chapter.

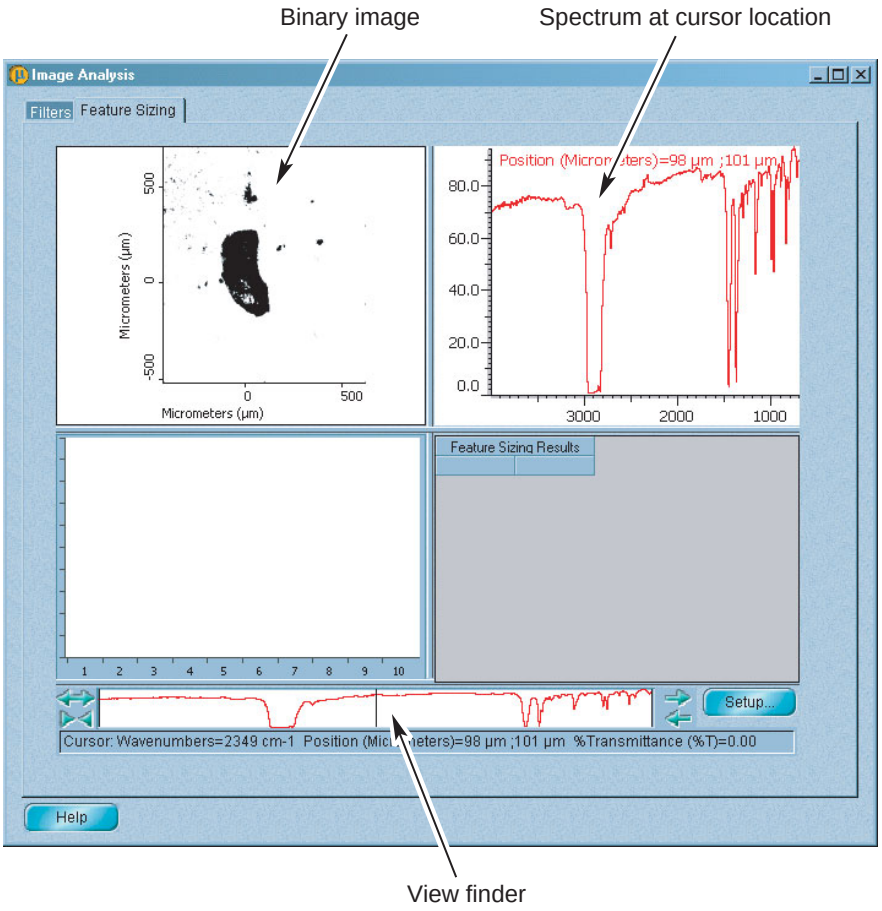
You can copy the image or either profile to the Windows Clipboard. Simply *right-click* the pane and choose Copy from the pop-up menu. You can then paste the copied item into programs that allow pasting from the Clipboard.

You can save the image or either profile as a .bmp, .jpg or .tif file by *right-clicking* the pane and choosing Save from the pop-up menu. Specify a file name, location and file type in the dialog box that appears and then choose Save. You can open the file later using a program that opens files of its type.

You can print the binary image, spectrum, histogram or results table by *right-clicking* the pane and choosing Print from the pop-up menu.

7. **Click the Feature Sizing tab.**

Here is an example:



The upper-left pane displays the binary image created using the settings you specified on the Filters tab.

The upper-right pane displays the spectrum collected at the current location of the cursor cross hairs in the image. You can move the cross hairs by dragging them or clicking a new location. The coordinate values of the current location appear below the view finder.

The bottom two panes will be used later to display the feature sizing results.

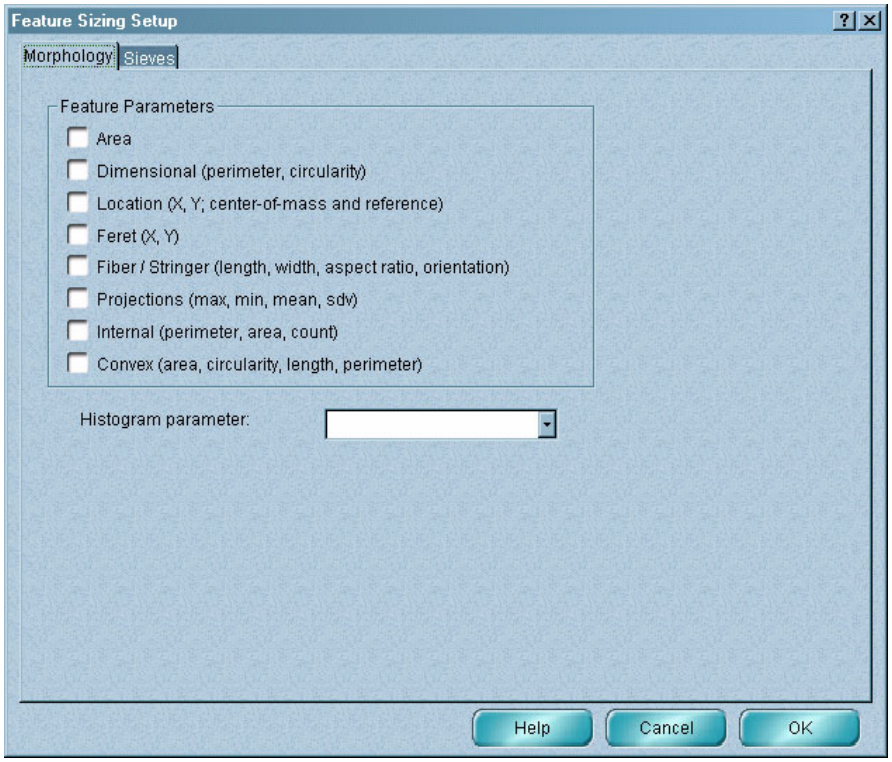
You can use the view finder to change the frequency limits just as you would in a map window. You can also change your view of the data by drawing a box on the image or in the spectral display pane and clicking inside the box, just as you could on the Filters tab. See the instructions in step 2 if you need help.

You can use a ruler to measure items in the image just as you could on the Filters tab. See the instructions in step 2.

You can save the binary image as a mask you can use when performing a principal component analysis. Simply right-click the image and choose Save Image As Mask from the pop-up menu. The mask remains in memory until you exit the software. See "Performing a principal component analysis" in the "Processing Map Data" chapter for more information.

8. Click the Setup button to specify the feature sizing measurements and sieves to use for the analysis.

The Feature Sizing Setup dialog box appears:

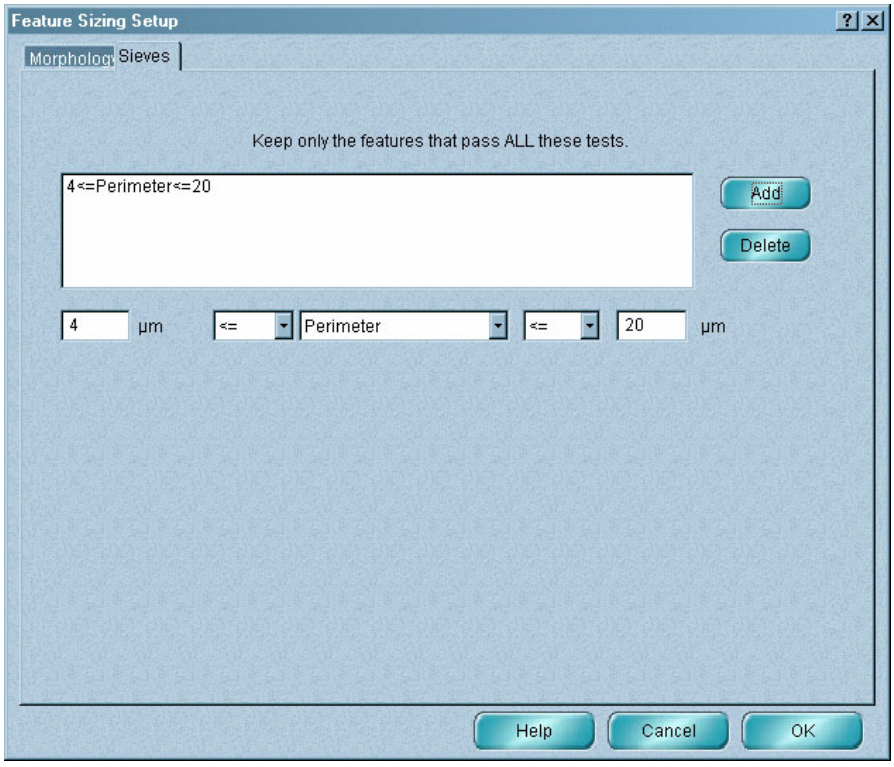


The Morphology tab lets you specify the feature sizing measurements to use for your analysis. In the Feature Parameters box select the parameters to include in the results table on the Feature Sizing tab of the Image Analysis window.

When you select a feature parameter, appropriate settings become available in the Histogram Parameter drop-down list box. Select the histogram parameter to plot in the histogram pane on the Feature Sizing tab. (You will be able to plot different parameters by clicking column headings in the results table on the Feature Sizing tab.)

See “Morphology options” earlier in this chapter for detailed descriptions of the available feature and histogram parameters.

The Sieves tab (shown below) lets you speed up the analysis by specifying one or more sieves that retain only those features that have certain characteristics. For example, you could specify a sieve to retain only those features whose perimeter is less than 4 micrometers or greater than 20 micrometers. Features must pass all the listed sieve criteria to be retained.



Follow these steps to specify each sieve you want to use:

a. Select a feature parameter from the center drop-down list box on the Sieves tab. These are the same parameters that can be selected from the Histogram Parameter drop-down list box on the Morphology tab. See “Morphology options” for detailed descriptions of the parameters.

b. Select the desired Boolean operators from the drop-down list boxes beside the feature parameter and enter values in the text boxes. Selecting a parameter determines the unit that appears, if any.

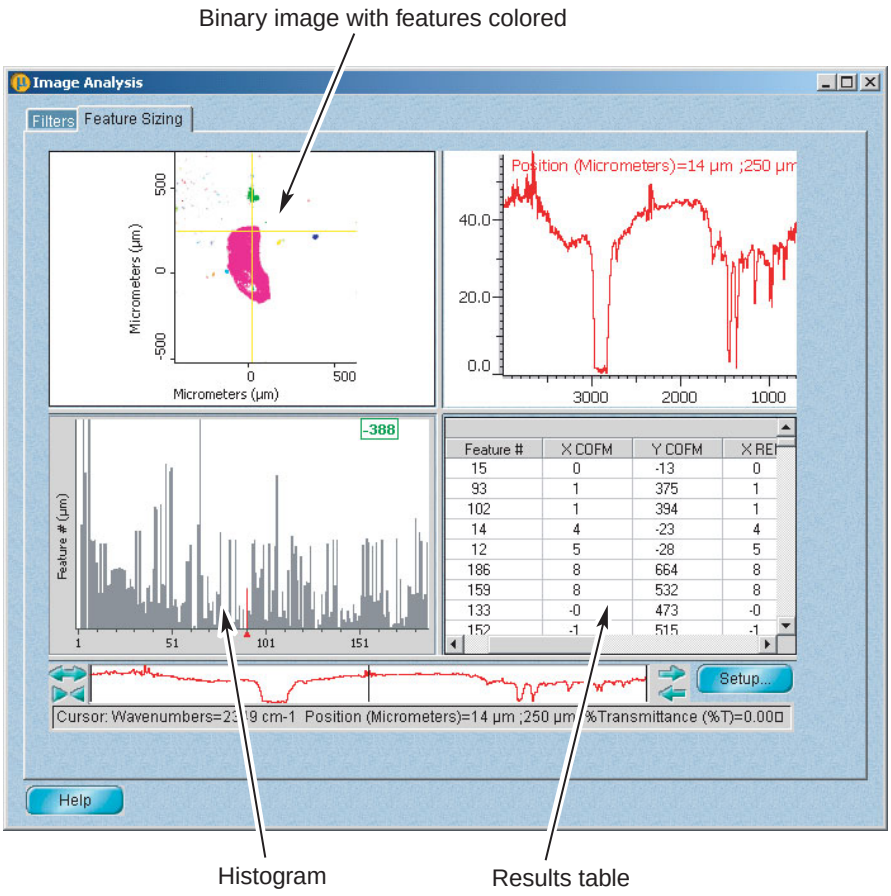
c. Click the Add button to add the sieve to the list.

Note Each feature parameter can have only one sieve. ▲

To delete a sieve, select it in the list and click the Delete button.

9. Choose OK to close the Feature Sizing Setup dialog box.

The analysis results appear on the Feature Sizing tab. Here is an example:



Each feature is assigned a consecutive number and displayed in a different color in the image. The numbers appear in the Feature # column of the results table.

Note If there are more than 16 features, the colors are reused in sequence as needed. ▲

For each feature the results table lists the results for the parameters you specified in the preceding step. Scroll bars are provided when needed to let you bring table columns or rows into view. When you click a cell in the table, the corresponding feature appears in red in the image.

To see a plot of the results for a particular parameter, click the appropriate column heading. The plot appears in the histogram to the left of the table. The X-axis of the histogram indicates the feature number; the Y-axis depends on the selected parameter. As you move the mouse over the histogram, the vertical bar at the current X value appears in green, and the Y value appears at the top of the pane.

You can copy the binary image, spectrum, histogram or results table to the Windows Clipboard. Simply *right-click* the pane and choose Copy from the pop-up menu. You can then paste the copied item into programs that allow pasting from the Clipboard.

You can save the binary image, spectrum, histogram or results table as a .bmp, .jpg or .tif file by *right-clicking* the pane and choosing Save from the pop-up menu. Specify a file name, location and file type in the dialog box that appears and then choose Save. You can open the file later using a program that opens files of its type.

You can print the binary image, spectrum, histogram or results table by *right-clicking* the pane and choosing Print from the pop-up menu.

10. To close the Image Analysis window, click the Close button (labeled "X") in the upper-right corner.

Saving and Exporting Map Data

This chapter explains how to save and export map data you have collected or processed.

Saving a map

Choose Save Map from the File menu to save the active line map, area map or depth profile. You can open the map later using Open in the File menu (see "Opening a map or files from a split map" in the "Opening and Importing Map Data" chapter).

If the map has not been saved before, the Save As dialog box appears. See the next section for instructions for using the dialog box.

To save the map with a different file name or in a different location, use Save Map As in the File menu. See the next section for details.

You can also export a map as an ENVI (*.DAT) file by using Export in the File menu, as explained in "Exporting map data."

Saving a map with a new file name or in a different location

Use Save Map As in the File menu to save the active line map, area map, depth profile, PCA results, quantitative analysis results, or the results of finding principal components using a different file name or location. You can open the map or other item later using Open in the File menu (see "Opening a map or files from a split map" in the "Opening and Importing Map Data" chapter). See "Performing a principle component analysis," "Quantifying a map" or "Finding component locations" in the "Processing and Analyzing Map Data" chapter for information about PCA analyses, quantifying a map or finding component locations, respectively.

Follow these steps:

1. **Choose Save Map As from the File menu.**

   The Save As dialog box appears.

2. **Type the desired file name in the File Name text box.**

   Use the extension .MAP.

Note If interferograms were saved when the map was collected, the name of the interferogram file will also be changed. (The "_IFG" portion of the file name will be retained.) See "Saving interferograms with the map" in the "Preparing for Data Collection" chapter for more information. ▲

3. **Locate and open the directory where you want the item saved.**

4. **Choose Save.**

Saving the current map background

Use Save Map Background, if available in the File menu, to save the current map background. See "Collecting an FT-IR or FT-Raman map background" in the "Collecting Map Data" chapter for information about collecting map backgrounds. Follow these steps:

1. **Choose Save Map Background from the File menu.**

   The Save As dialog box appears.

2. **Type the desired file name in the File Name text box.**

   Use the extension .SPA.

3. **Locate and open the directory where you want the background saved.**

4. **Choose Save.**

Exporting map data

Use Export in the File menu to save the map displayed in the active map window as an ENVI software file. Follow these steps:

1. **Choose Export from the File menu.**

   The Save As dialog box appears.

2. **Type a file name in the File Name text box.**

3. **If you want the map exported to a different directory, locate and open that directory.**

4. **Choose Save.**

Printing

This chapter explains how to print a map window or profile window, items displayed in a map window and Mosaics. If you have not already selected and set up a printer, use Printer Setup in the File menu before printing. In OMNIC Help Topics find "printer" in the Index and go to "Setting up the printer" for more information.

Printing a map window, profile window or quant results window

Use Print in the File menu to print the active map window, profile window or quant results ("Quantify") window, with its currently displayed panes. You can use Options in the Edit menu to specify how to print the window; for example, whether to print the panes on separate pages. See "Specifying how to print map windows" in the "Preparing for Data Collection" chapter for details.

You can also print individual panes of the window. See "Printing items displayed in a map window" for details.

Note To print a Mosaic of video images displayed in the navigation pane, use Print Mosaic in the Atlμs menu as explained in "Printing a Mosaic." ▲

Follow these steps to print the active map window or profile window:

1. **Choose Print from the File menu.**

   The Print dialog box appears.

2. **Set the print parameters as desired.**

3. **Choose Print.**

Printing items displayed in a map window, profile window or quant results window

Follow these steps to print an individual item displayed in a map window, profile window or quant results window:

1. ***Right-click*** **the item you want to print.**

   You can print the contour map (or discrete point location map), video image, spectral display pane and 3-D image.

2. **Choose Print from the pop-up menu.**

   The Print dialog box appears.

3. **Set the print parameters as desired.**

4. **Choose Print.**

Printing a Mosaic

After you have used Capture Mosaic in the Atlμs menu to display a Mosaic of video images for a sample area, you can print the Mosaic, along with the navigation pane axes, on paper by using Print Mosaic in the Atlμs menu. See "Capturing a Mosaic of video images for a sample area" for more information on displaying a Mosaic in the navigation pane.

Follow these steps to print a Mosaic:

1. **Choose Print Mosaic from the Atlμs menu.**

   The Print dialog box appears allowing you to set the parameters for printing.

2. **Set the parameters as desired.**

3. **Choose OK.**

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